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Methodology for Estimating Direct Exposure to New Chemical Substances

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16. ABSTRACT

The Toxic Substances Control Act (TSCA) requires each person who intends to manufacture a new chemical to submit a Premanufacturing Notice to the EPA at least 90 days before manufacture commences. The work reported here was directed toward the development of a procedure for the orderly and rapid prediction of direct human exposure which might result from such manufacture. The procedure developed involves the following steps: (1) prediction of unavailable physical and chemical properties from analogs and general chemical knowledge, (2) prediction of production volume based upon company size, current markets and total market volume, (3) prediction of chemical operator exposure and exposures in the vicinity of the plant based upon fugitive emissions and (4) prediction of consumer exposure based upon active use and passive use of the chemical.

The procedure will permit rapid screening however further refinements will enhance the usefulness.

17. KEY WORDS AND DOCUMENT ANALYSIS

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FOREWORD

This study was conducted for the Pre-manufacturing Review Division, Office of Toxic Substances, Environmental Protection Agency, (EPA), to collect data and develop procedures for the assessment of direct exposure as an integral part of the risk assessment scheme for new chemical substances. It focused primarily upon the initial screening of new chemical substances. However, this study is not limited to new chemical substances; the methodology and procedures described are sufficiently broad to be useful to other EPA programs.

This document was published with the expert advice of Dr. James Falco, Office of Research and Development, and Dr. Peter Voytek and Mr. Stuart Cohen, Office of Toxic Substances. Further information can be obtained from the Pre-manufacturing Review Division; telephone: 202-426-2601; address: Office of Toxic Substances (TS-794), U.S. Environmental Protection Agency, 401 M Street, SW, Washington, DC 20460.

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SECTION 1

INTRODUCTION

PREMANUFACTURING NOTIFICATION REQUIREMENTS

Section 5 of the Toxic Substances Control Act (TSCA) requires each person who intends to manufacture a new chemical substance for commercial purposes to sumbit a notice to EPA at least 90 days before manufacture commences. At the end of the notification period the person may manufacture the substance unless EPA has taken regulatory action under section 5(e) to request additional data or under section 5(f) to ban or otherwise regulate the substance.

Section 5(d)(1) of TSCA requires the manufacturer to report chemical identity, uses, and exposure data. In addition, the submitter must provide all test data related to the effects on health and the environment of the manufacturing, processing, distribution in commerce, use, and disposal of the new chemical substance to the extent they are known to or reasonably ascertainable by the submitter.

On January 10, 1979, the EPA published proposed rules and notice forms in the Federal Register, and subsequently held a series of public meetings throughout the country to obtain written and oral comments on the proposed rule making. On May 15, 1979, EPA published its Interim Policy for the premanufacture program applicable until the Agency promugates its final rules and forms. Also, in September, EPA reproposed the notice forms for further public review and comment.

EPA also published three documents with this proposal:

> Support Document, Premanufacturing Notification Requirements and Review Procedures, Office of Toxic Substances Washington, DC, January, 1979.
>
> Explanatory Appendix, Premanufacturing Notice Forms, Office of Toxic Substances, Washington, DC, January, 1979.
>
> Impact of TSCA Premanufacturing Notification Requirements, Office of Toxic Substances, Washington, DC, 1979.

GENERAL APPROACH

EPA's implementation of Section 5 of TSCA will focus upon the assessment of risks associated with the manufacture, processing, distribution in commerce, use, disposal of new substances. This risk assessment will involve developing estimates of both the potential extent of human exposure and potential toxicological effects on human health and the environment for each new chemical. Possible risks then can be balanced against economic and other non-risk factors in order to evaluate the reasonableness of the risks.

RESTRICTIONS AND LIMITATIONS

The number of new chemicals which will have to be evaluated each year has not been determined as of this time. Estimates have ranged from as low as 150 to as many as 1,000. Since one major company states it will attempt to commercialize 100 new polymers and oligomers per year, it would seem that the higher estimate will be more realistic.*

The submissions must be acted upon within 90 days and preferably within a shorter period.

The manufacturer must supply the information which is know to him or is reasonably ascertainable. It is expected that many manufacturers will be able to supply only limited information in their notices and that EPA make decisions that are be as definitive as possible based upon this limited information.

PURPOSE AND SCOPE OF THIS EFFORT

The purpose of this study was primarily to elaborate procedures for making direct exposure assessment and was particularly directed toward the initial screening operation. This involved identifying relevant parameters of exposure, determining the priority for consideration of these parameters, developing specific quantitative data and test results for direct exposure based on the literature, and developing a background for the use of structure-property relationships.

EPA's Office of Toxic Substances has limited resources for the formulation of decisions on new chemicals. The purpose of this program was to develop procedures and data which could permit rapid assessment of direct exposure and which could become an integral part of the unreasonable risk assessment scheme for new chemicals.

It was fully recongnized that the exposure assessment procedures would be qualitative in nature and, at the optimum, would result in general categories or ranges describing the degree of the exposure. Nevertheless numerical methods were used throughout.

---

*Wismer, M., Let's Reason Together and Simplify PMN, Chemical Week, May 16, 1979, p. 5.

To accomplish these objectives the effort was divided into the following tasks:

- Development of a procedure for prdicting exposure during manufacture and processing;
- Development of a procedure for predicting exposure during consumer use;
- Development of a procedure for predicting production volume for the third and fifth years;
- Study of the relationships of chemical and structure to physical, chemical and biological properties, and
- Application of these procedures to candidate compounds.

SECTION 2

SUMMARY

Assessment of unreasonable risks during the production and use of new chemicals requires consideration of toxicity, exposure, and economic factors. This effort involved the development of concepts and procedures to predict the direct exposure during manufacture, processing and use of a new chemical. The effort was based upon the premise that there would be very little information as to the physical or chemical properties of the new chemical, and only limited information concerning processing steps, production volume, anticipated growth in production, and potential uses. In spite of these limitations it is necessary to rapidly screen perhaps as many as 1,000 chemicals per year and to separate those chemicals which represent very little exposure from those that have the potential for high exposure.

The approach developed utilizes the following steps:

ESTIMATION OF PHYSICAL AND CHEMICAL PROPERTIES IMPORTANT TO DIRECT EXPOSURE

Limited physical and chemical data will be available for some candidates and it will be necessary to estimate properties such as vapor pressure, octanol-water partition coefficient, chemical stability and possible uses based upon the chemical structure of the compound. The techniques for preparing such estimates are discussed.

ANALYSIS OF PROJECTED USES AND PREDICTION OF PRODUCTION GROWTH RATES

Evaluation of exposure assessment due to manufacturing and consumer use requires estimation of production volume for the first, third and fifth years of production. EPA proposed to request this information on the PMN forms. However the confidential nature of this information and the possibility that the form would be modified to delete these estimates made it advisable to independently predict the production volume and the use categories. A method of production estimation based upon use categories and data concerning the applicant company has been developed.

CALCULATION OF EXPOSURE OF MANUFACTURING PERSONNEL AND POPULATIONS IN NEAR PROXIMITY TO THESE PLANTS

Exposure of production workers can be estimated based upon fugitive losses, plant size, ventilation rates, and production volume. The number of workers exposed and the concentration of the chemical in the air can be predicted for normal chemical plant operations.

Fugitive losses have been used as source strength to calculate exposure of populations in the vicinity of the plant.

PREDICTION OF ACTIVE AND PASSIVE EXPOSURE DURING CONSUMER USE

A procedure for estimation of the dose of the chemical recieved by a consumer whether by inhalation, ingestion or skin adsorption in either the active or passive phase of the use has been developed along with guidelines for estimating the total fraction of the population involved.

The approach developed was used to calculate exposure from 30 chemicals which differ with respect to production volume, physical and chemical properties, and uses.

The procedure appears to be satisfactory, however, it does require the use of technical judgement during each phase of the analysis.

It is recommended that the procedure be adopted on an interim basis and that efforts to refine the data bases and procedure be continued.

EXPOSURE ASSESSMENT PROCEDURE

The procedure developed during this effort can be used to estimate exposure during manufacture, processing and use. The procedure is general in the sense that it does not require site-specific information, details on the processing steps, details as to equipment to be used and only limited data as to physical or chemical properties. If this information is available, it will increase the accuracy of the prediction; however, even without these data a first level estimate of exposure can be made. The procedure is directed toward conditions of normal chemical production and normal usage, it does not address the case of poor equipment or plant design, accidental spills or misuse of the consumer product.

This report presents the procedures for prediction of exposure during the manufacture, processing and consumer use of a new chemical. Since the information for these predictions may or may not be available from the Premanufacturing Notice (PMN) forms it was believed necessary to provide procedures for the estimation of critical data such a possible growth in production volume and those physical, chemical and biological properties which may affect exposure.

SECTION 3

PREDICTION OF EXPOSURE DURING MANUFACTURE AND PROCESSING

Plant operating personnel will probably be exposed to the highest concentration of any new chemical. Regulation of this exposure is a joint EPA/OSHA responsibility, however, the OTS could make a preliminary assessment of exposure and then alert OSHA to any potential problem.

In order to accomplish this mission, the OTS will conduct a preliminary assessment of exposure based upon information supplied in the PMN and upon accepted industrial practices. A conservative approach must be taken to insure adequate regulation of new chemicals. Thus in the evaluation a "normal" and "worst case" should be evaluated.

While data specific to the particular production facility may be available, the evaluation should not be specific to a particular site or set of conditions.

In the following sections the rationale for the numbers used in calculating exposure is presented. Literature references are cited where available and where project personnel exercised engineering judgement, it is so indicated. Periodicals and books devoted to chemical production were searched up to date; however, many of the most useful articles were published several years ago. These references were used if, in the judgement of the project engineers, they were representative of current conditions.

The method used to estimate exposure during manufacture or processing utilized the following parameters:

Source Strength:	as a fraction of production
Building Size:	as a function of production
Ventilation Rate:	as 10 changes per hour
Workers Exposed:	as a function of production volume and number of processing steps

The exposure of people in the vicinity of the plant was estimated using a fraction (0.001) of production as the source strength and a diffusion model.

PRODUCTION RATE

The annual production rate is requested in the PMN forms and will be provided by the applicant. A simple annual production figure could be misleading and further details may be necessary. Many specialty chemicals are produced in existing facilities rather than in facilities designed specifically for the chemical. This results in mis-match of production rates and equipment capacities such that some unit processes may be utilized only a small fraction of the time while others are used continuously. In other cases the total annual volume could be produced in a 30 or 60 day period. This would result in exposure of plant operators to a much higher concentration than would be calculated based upon annual production and 250 days of operation.

Since we are concerned with the introduction of a new chemical there are some economic constraints imposed upon the production volume. It is expected that the volume produced would be sufficient to provide test marketing information. For some chemicals only a few hundred pounds are required for a test market whereas with others several thousand pounds are required. For example, a chemical used to produce urathane foam, might require as much as 6,000 lbs for production tests and product evaluation. Another chemical used in an insecticide formulation may require less than 200 lbs. Generally a few thousand pounds are required for test and evaluation. It is expected that the annual production listed in the PMN forms will vary from 1,000 to 100,000 lbs/yr.

PROCESS LABOR REQUIREMENTS

The chemical process industries typically have had a low labor/unit production requirement. This results from automated and large scale operations. The relationship of the labor requirements to the production volume has been described by the "2 tenths factor rule."[1] An example of this rule is given below.

A chemical plant is operating with 600 man-hours per week and a production volume of 100,000 lb/day. If the production is increased to 500,000 lb/day, how many man-hours would be required?

$$\text{man-hours} = 600\left(\frac{500,000}{100,000}\right)^{0.2} = 828 \text{ man-hours}$$

Thus an increase of only 38% in labor is required for a 500% increase in production.

C. H. Chilton[2] gave some typical process labor requirements. These show a range of from 0.2 to 80 man-hours/ton of product. Included in his article are high and low volume chemicals and chemicals that require little to extensive processing. The majority of operations fall in the 1-10 man-hours/ton of product range. While these figures are informative they are not well suited for use in a model to be used for prediction of labor requirements.

A more useful model is described by Wessel.[2] The plant capacity is used to estimate the labor requirements per ton of product per process step. This is shown graphically in his article and in Figure 1. This method is the most general and is incorporated into the exposure model.

In general process labor increases as the production increases and as the number of steps increases. As the production volume increases beyond some point it becomes more economical to use a continuous rather than a batch

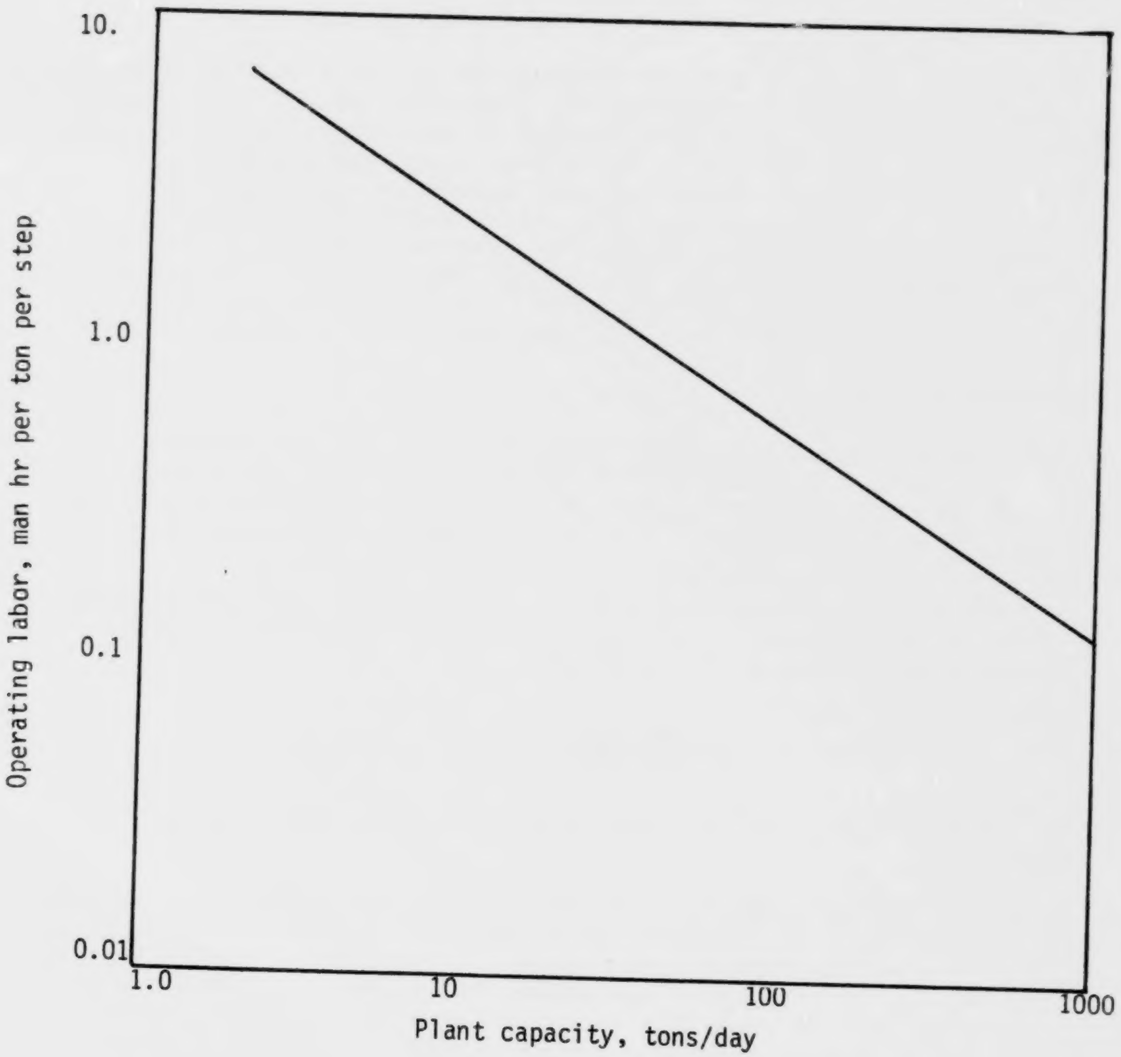


Figure 1. Labor requirements as a function of plant capacity (from Wessel[2]).

process. The decision of batch versus continuous processing is dependent upon factors such as availability or cost of equipment, production rate, number of process steps, number and size of recycle streams and labor requirements. It is expected that the majority of new chemicals will be initially manufactured by batch processes.

MANUFACTURING SOURCE STRENGTH

The procedure proposed to evaluate exposure of manufacturing plant personnel requires an estimate of the amount of product lost during manufacture or processing. These losses occur due to leaks in pipe joints, gaskets in piping or reactors, pump seals, vent streams, wash-down during maintenance, minor spills, etc. These losses may range as high as 3% of the total production.

An attempt was made to categorize the allowable concentrations in the air at the work place and to relate these concentrations to the physical properties (i.e. vapor pressure) of the chemical. This effort did not result in any useful relationships. It appears that the level of contamination in a plant is more related to worker discomfort or toxicity constraints than to the physical or chemical properties of the chemical. In other words, the concentration of chemical in the plant depends upon good design, good maintenance and good housekeeping and not upon the properties of the chemical.

An example of this hypothesis is the manufacture of vinyl chloride polymers. When there were no restrictions upon the operations the plant personnel (and the surrounding neighborhoods) were subjected to high concentrations. With current restrictions the concentrations in the plant are below the OSHA limit of 1 ppm (8 hr TWA). This change has been the result of new designs and new operating procedures.

An attempt was made to accumulate sufficient information to predict emissions to air, land, and water from chemical production facilities based upon the process unit operations involved in the manufacturing process. As a result of a literature review and several telephone conversations with EPA staff, it was discovered that there is very little published data in this area. The U.S. EPA, Chemical Manufacturing Section: Chemical and Petroleum Branch; Emission Standards and Engineering Division; Office of Air Quality Planning and Standards; U.S. EPA: Research Triangle Park, is currently involved in a program to generate this data, however, it will not be available until mid 1980. The work is concerned with air emissions. No water and/or land emissions data or research efforts were found.

EPA Report No. 560/1-77-002[3] lists the three levels of emission categories shown in Table 1. These values were apparently estimates based upon the authors' knowledge of the industry and are not supported with any measurements. These categories incorporate dispersion emissions from product intermediate and end use as well as emissions from manufacturing operations.

TABLE 1. ESTIMATED EMISSION FOR THREE CHEMICAL CATEGORIES

Low Emissions	0-3%	Chemicals manufactured for in-plant use.
Medium Emissions	3-50%	Chemicals which are not destructively consumed at manufacturing site.
High Emissions	100%	Chemicals which are dispersed to the environment (i.e. aerosols).

The data in EPA Report 450/3-77-008a[4] contains emission factors as a percent of total production. These are assumed to be 1.5% when no data were available. The range of emissions reported in this reference varied from 0.7% for hexanol to 3% for several compounds. There is no apparent correlation between the emission values and the physical properties of the substance.

The EPA has studied the manufacture of several individual chemicals for purposes of exposure assessment. Reports on ethylene dichloride, ethylene dibromide, benzene, and vinyl chloride contained emission figures for the manufacture of these chemicals.[5,6,7,8]

Ethylene dichloride and ethylene dibromide were assumed to be emitted at 1.5% of production, benzene emissions were estimated at 0.5% of production. Vinyl chloride emissions are shown in Table 2.

TABLE 2. VINYL CHLORIDE EMISSIONS
(FOR ETHYLENE DICHLORIDE-VINYL CHLORIDE PROCESS)

Source	VCM Emissions kg/100 kg (lb VCM/100 lb) VCM
Fugitive	0.1215
EDC Finishing Column	0.05
VCM Finishing Column	0.24
Oxychlorination Process	0.0364
Process Water	0.007
TOTAL	0.4479

This shows a total emission of 0.4479% or approximately ½% of vinyl chloride monomer produced.

The U.S. EPA compiled a list of Air Pollution Emission Factors in Report AP-42.[9] This report has a discussion of the emissions from a number of chemical manfuacturing operations. As was noted in the report, these figures were often estimated from yields or material balances since little emission data were available. The emissions are categorized into raw material, intermediate, by-product, and product emissions thus making these data the most specific of the information available at this time. Emission factors for total emissions in controlled situations varied from 0.01% to 8% of the production volume. The major factor influencing emissions was the emission control devices applied. This report is the most useful of the available published government documents on emission factors.

Emissions from the top 139 organic chemical manufacturing operations were obtained from Emission Standards and Engineering Division. They list as the source of their data as State EIQ's, Monsanto Research Corporation, Radian, Houndry, site visits and product reports. Emissions ranged from 0.0007 lb/lb product for linear alkyl sulfonate to 0.1098 lb/lb product for acrylonitrile and hydrogen cyanide. The majority of emissions are less than 1% with a considerable number of emissions in the 0.1-0.5% range. This report shows several other interesting items as well, including the various processes used to manufacture the chemical, gross emission, predicted growth rate, and toxicity rank.[10]

Another EPA program characterized production emissions into four categories:[11]

Process Vents
Fugitive
Storage and Transportation
Solid and Liquid Waste Emissions

Values for the percent of total emissions in each category is given in Table 3. Process vents and fugitive emissions account for the majority of the total emissions.

TABLE 3. RELATIONSHIP OF EMISSION ROUTES

Emission Route	% of Total Emissions to Air
1. Process Vents	66-70%
2. Fugitive Emissions	15-20%
3. Storage and Transportation	8-10%
4. Solid & Liquid Waste Stream Emissions	2-5%

An excellent discussion on the problems associated with characterizing and controlling the emissions from chemical manufacturing facilities is presented by David Patrick in "The 2nd Year End Report: Synthetic Organic Chemical Manufacturing Industry Standards Development Program."[12] This report is not released for public distribution but was obtained upon request.

Emissions generated by new chemicals are not expected to exceed the highest reported values in the above mentioned literature. With the use of appropriate controls, fugitive emissions should range from 0.1 to 0.6% of production. The fact that many chemical substances are produced with less than 0.5% emissions indicates that this emission range is reasonable and could be attained in a properly designed manufacturing facility.

The fugitive emission rate for a reasonably volatile new chemical manufactured using conventional design and precautions has been assigned a value of 0.1% of production rate. A high value of six times this or 0.6% has been assigned to represent the case where few precautions are taken to protect the worker.

The above data apply to the case where the emission is volatilized into the air at or shortly after the leakage point; a somewhat different situation applies when the emission is a non-volatile material.

If the fugitive emission is in the form of particulate matter, it should be treated somewhat differently than a vapor or gas. The vapor or gas would be expected to leave the work place with the ventilating air whereas the particulate matter may accumulate on such places as equipment, floors, building surfaces, and operator clothing. The degree of accumulation is again dependent upon plant design, operating procedures and housekeeping practices.

Particles below 5 μm would be expected to remain airborne and to be removed with the ventilation air. Larger particles may well settle on surfaces within the plant. Personnel would be exposed to some higher, but unknown, level than is indicated by the fugitive emission losses. This level would be dependent upon housekeeping, perhaps water solubility, color, degree of irritation and upon the types of processes such as ball milling, conveying, blending, packaging, etc.

Many plants operate with a weekly wash-down schedule and such a schedule is assumed here. Based upon these considerations, the source of non-volatile fugitive emissions is taken as 3x the amount given as a percentage of production or 0.3% of the production rate for the normal case and 1.8% of the production rate for the case were minimum precautions to protect the worker are taken.

VENTILATION RATES

Ventilation of process buildings is used to remove odors, toxic chemicals, and excess heat. Ventilation design depends upon the specific process and quite often local ventilation will be used rather than total building ventilation to accomplish these purposes. However, for the purposes of the exposure model a different approach was required in that the number of air changes per hour for the total plant are needed.

The American Iron and Steel Industries report a general ventilation rate in steel plants of about 2 $ft^3/min\ ft^2$.[13] Using a ceiling height of 14 ft this gives a ventilation rate of 8.6 air changes per hour. This is a reasonable figure and close to the expected range based upon the experience of the IITRI staff.

The Code of Federal Regulations (1978)[14] requires a ventialation rate of 1 cfm per square feet of floor area for processing buildings using Class I liquids. This includes flammable or combustible liquids and operations such as mixing, drying, evaporating, filtering, distillation or similar operations "for example in compounding of cosmetics, pharmaceuticals, solvents, cleaning fluids or insecticides."

A ventilation rate of 10 air changes per hour was selected for use in the exposure model based upon the above and other publications.[15,16]

BUILDING SIZE IN THE CHEMICAL PROCESS INDUSTRIES (ENCLOSED PLANTS)

The size of enclosed chemical process plant buildings in one of the factors entering the worker exposure model. It was assumed that any new chemical would be produced in an enclosed facility. This is a worst case situation since many chemical plants, especially large ones are constructed outdoors with only portions of the equipment and the controls indoors.

A model predicting building size based upon production capacity would be ideal, however, no such data were found in the literature. A search of the literature did reveal an estimated building size for typical enclosed production facilities. The author quotes a typical building size a "65-95 ft in width and 150-250 ft in length with few exceptions."[17] Allowing a ceiling height of 13 ft and 2-3 floors gives a range in building size of 250,000-925,000 ft^3.

Since the production volume is expected to relate to the plant size, the following model is proposed.

The range of sizes, 250-925 thousand ft^3 (7 to 26 thousand m^3) is assumed to be linearly proportional to the production volume in the range 1,000 to 10,000 lb/day (450 to 4500 kg/day). A graph of this relationship is given in Figure 2. Sizes outside this range can be determined by extrapolation.

ASSESSMENT OF EXPOSURE DUE TO PROCESSING

Exposure during the processing of the chemical can be estimated in a manner very similar to the procedure used for the estimation of exposure during manufacture.

In many instances the new chemical is chemically or physically combined with other materials to produce a product. For instance, pigments are physically combined with solvent and binder to make paint, and dichloroethylene is chemically modified to make a new product, vinyl chloride.

The source strength is considered to be the fraction of the new chemical in the processed product times the amount of the new product and the estimation of exposure proceeds in the same manner as was used for the manufacture of the chemical.

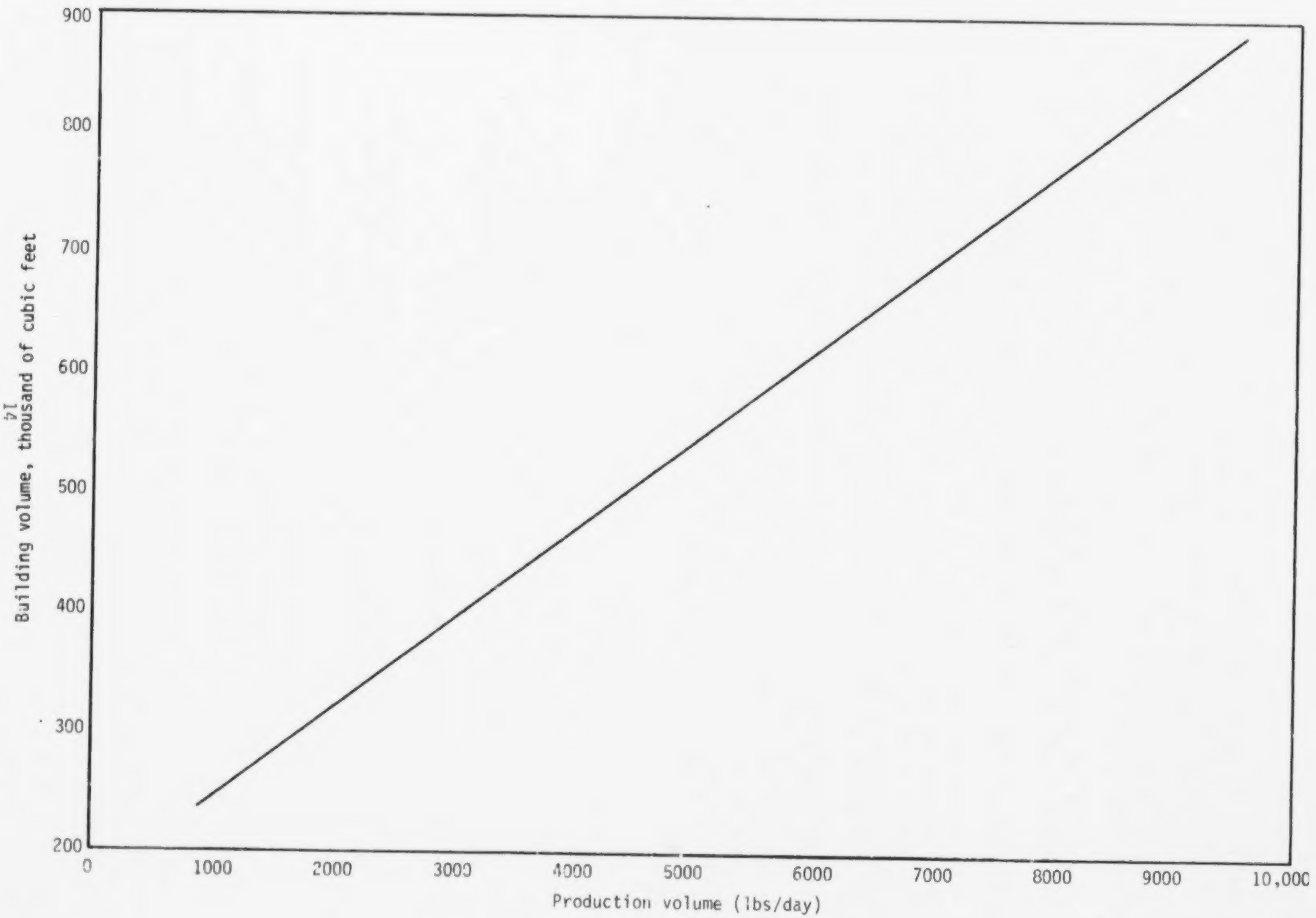


Figure 2. Building size vs. production volume.

TRANSPORTATION EMISSIONS

Emissions originating from the transportation of chemicals depends on the equipment and emissions controls used, the physical state of the chemical, and the vapor pressure of the chemical. The predicted emissions from the transport of volatile organic liquids were prepared and will soon be reported by the U.S. EPA. A preliminary copy of the final report on this subject was obtained from the Emission Standards and Engineering Division, Office of Air Quality Planning and Standards. An emission factor for new chemicals can be derived from this information based upon the vapor pressure of the chemical of interest. These factors are given below in Table 4.

To date, transportation losses have not been considered in the exposure model.

TABLE 4. LOADING AND TRANSPORTATION EMISSION FACTORS

Vapor Pressure, KPa*	Loading Loss Kg Lost/Kg Produced	Transportation Loss Kg Lost/Kg Produced	Total kg Loss Kg Produced
0.001- 6.9	0.0000199	0.00000354	0.0000234
1.4 - 3.5	0.00006999	0.0000125	0.0000825
3.5 - 6.9	0.000124	0.0000271	0.000151
6.9 - 10.3	0.000187	0.0000453	0.000232
10.3 - 20.7	0.000299	0.0000814	0.000380
20.7 - 34.5	0.000399	0.000144	0.000543
34.5 - 51.7	0.000622	0.000226	0.000849
51.7 - 69.0	0.000872	0.000317	0.00119
69.0 -103.4	0.000995	0.000361	0.00136
Above 103.4	Negligible (Closed System)	Negligible (Closed System)	Negligible

*kilopascals (mm Hg)

ASSESSMENT OF EXPOSURE IN THE PLANT VICINITY

Turner's Gaussian plume model was used to estimate, within an order of magnitude, average concentration in an area around a point source of effective height H, emitting at a steady rate of Q gms/sec.[18]

The following assumptions were made:

Basis:

- All calculations were based on uniform atmospheric stability, class D.
- Average wind speed, U, equals 5.5 m/sec.

- There are no "prevailing wind" directions, the wind blows at the average speed for equal interval of time from each of the 16 compass directions.

- The point source emits at a steady, uniform rate of Q gm/sec.

Then Turner's equation for average concentration $\overline{X}$ becomes:

$$\overline{X} = \frac{2.03\ Q}{\sigma z U x} \exp\left[-0.5\left(\frac{H}{\sigma z}\right)^2\right]$$

$$\text{or } \frac{\overline{X}\ U}{Q} = \frac{2.03}{\sigma z x} \exp\left[-0.5\left(\frac{H}{\sigma z}\right)^2\right]$$

where Q = source strength gm/sec

U = wind speed, m/sec

X = distance, m

H = effective plume height, m

σz = standard deviation of plume concentration distribution in vertical direction, m

Consideration has been given to the exposure of the general population in the vicinity of manufacturing or processing plants. Atmospheric diffusion models can be applied to gases or the very small particles which remain airborne. The simple models do not account for deposition of particles or reaction of the gases or vapors. The simple model was considered to be sufficiently accurate for the predictions required for preliminary evaluation.

Plots of this equation for two values of H are illustrated in the Figure 3. This figure may be used to estimate the radius of a circle in which the average pollutant concentration is $\overline{X}$, released from a point source at effective height H, emitting at a steady rate Q.

Generally, for short sampling time (∿2 hrs), Turner's model is expected to be within a factor of 2 to 3. However, in attempting to estimate long term, yearly averages the accuracy would rapidly decrease and would probably be within 2 to 3 orders of magnitude.

Effective Stack Height H

Effective stack height H is the sum of stack height (HH) and plume rise (ΔH). Plume rise is defined as the distance between the top of the stack and the axis of centroid of the pollutant distribution. It has been found to be dependent upon exit velocity of stack, diameter of stack, mean wind (horizontal) speed, atmospheric stability class, lapse rate and the temperature difference between the stack gases and ambient air.

There are numerous plume rise formulae. Most of these are semi-empirical. For a review of these see Moses, Strom, and Carson.[19]

An empirical equation was presented by Holland which may be used to estimate ΔH. This equation frequently underestimates the effective height of emission, therefore, it often provides a slight "safety" factor.

Hollands equation is:

$$\Delta H = \frac{Vsd}{U}\left(1.5 + 2.68 \times 10^{-3} p \, \frac{Ts - Ta}{Ts} \, d\right)$$

where ΔH = rise of the plume above the stack

Vs = stack gas exit velocity, m/sec

d = inside stack diameter, m

U = wind speed, m/sec

p = atmospheric pressure, mb

Ts = stack gas temperature °K

Ta = air temperature °K

and 2.68×10^{-3} is a dimensional constant having units of $(mb)^{-1}m^{-1}$. From Figure 3 it is apparent that the more conservative estimate would utilize $H = 0$. For the purposes of estimation of population exposure it is suggested that the stack height plus plume rise be considered as equal to zero. The worksheets for exposure in the vicinity of the plant are based upon $H + \Delta H = 0$.

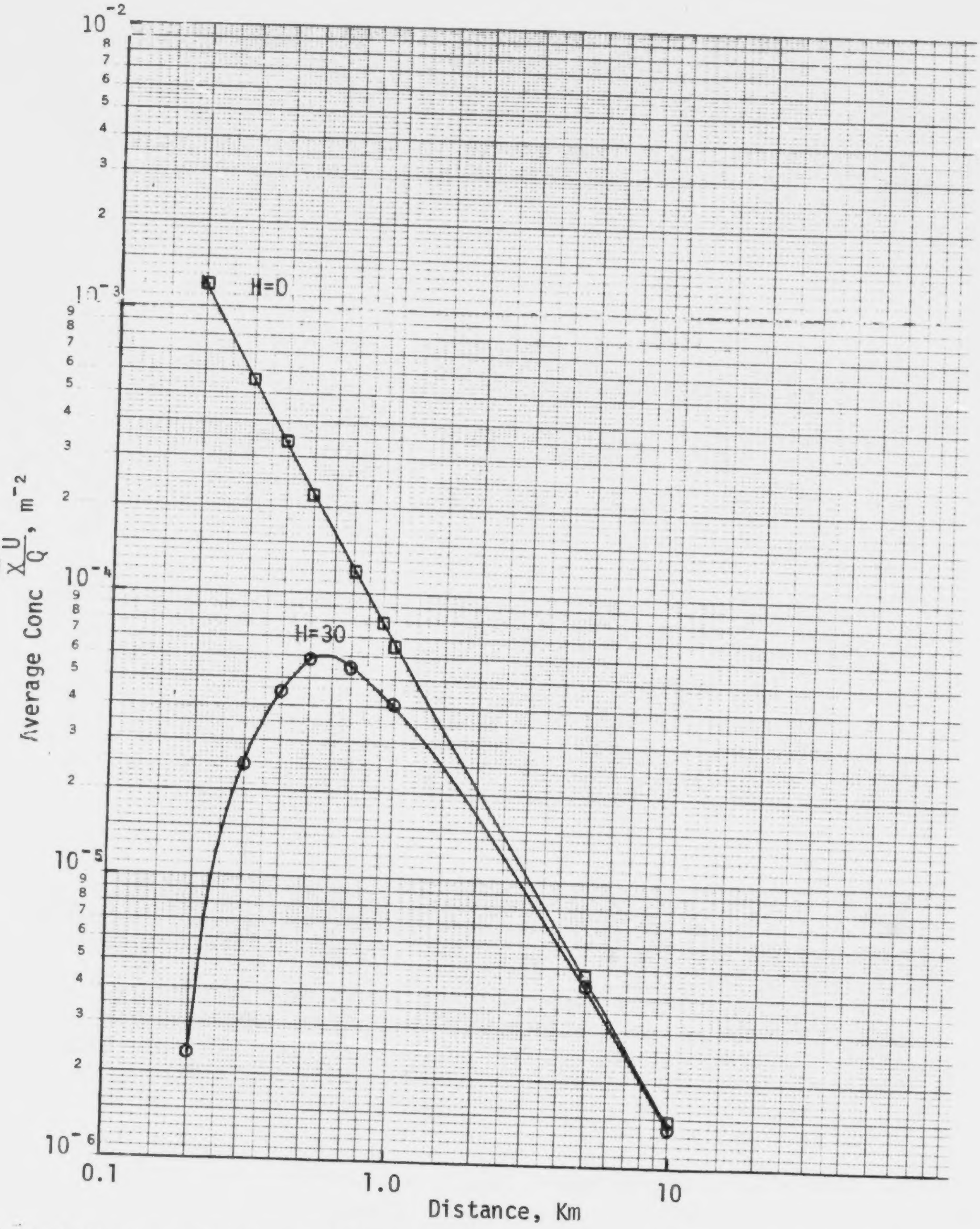
Population Density

The number of people exposed to chemical emissions is a function of the population density near the emission source. Source-specific information can be derived from Census Bureau Information.

A more general model was sought since information as to the specific manufacturing location may not be available or may change after the chemical goes into production. Three sources of population density statistics were selected and used to derive a best estimate average population density for typical manufacturing sites.

The first source of population density was obtained from EPA CRESS Report No. 39 (July, 1978).[20,21] The range of population densities for cities with plants manufacturing ethylene dibromide was from 552-1604 people/km^2.

The second source of population density data was obtained from U.S. EPA 450/2-75-009, a report on exposure to vinyl chloride.[22] Data presented in



$\bar{\chi}U/Q$ with Distance for Two Heights of Emission (H in Meters), Class D Stability

Figure 3. Ambient air concentration as a function of distance from the source.

this report indicate an average population density of 388 people/km^2 within a radius of 5 miles of vinyl chloride and polyvinyl chloride production facilities.

The third and most detailed general population density data were obtained from U.S. EPA CRESS Report No. 27 on coke oven emissions.[23] Average population densities at several distances from 65 coke plants were calculated and are given below.

Distance From Coke Plant (Km)	Population Density (People/km^2)
0.0 - 0.5	641
0.5 - 1.0	757
1.0 - 3.0	1006
3.0 - 7.0	885
7.0 -15.0	618

Selecting the population density to be used in the exposure model was basically a matter of engineering judgement. Note, however, that the range of population densities noted above is from 388-1604. The maximum density is thus only a factor of 4 larger than the smallest. A population density of 3 times the minimum or 1164 people/km^2 was chosen. It is believed that this figure represents the high side of the expected population densities. However, this figure was chosen so that the model will tend to slightly overestimate and not underestimate the number of people likely to be exposed to emissions from production and processing facilities.

Routine Estimations

The estimation of exposure due to manufacturing and processing can be simplified and requires only a very short time for any one particular compound and site. Forms for such calculations and an example are shown on the following pages.

MANUFACTURING EXPOSURE

CHEMICAL:

NO. __________

Annual Production, P, ________________________________ kg/yr

Number of Plants, N, ________________________________

Number of Days in Production, D, ________________________

Number of Process Steps, S, ___________________________

Persistence, R, Gas = 1.0 Nonvolatile = 3.0

Maximum Daily Production Pmd __________________________ kg/day

In-Plant Concentration, normal operations, Cn =

$$Cn = \frac{(4.167)(R)(Pmd)}{(4.67)(Pmd)+5660} =$$

Number of workers exposed, W,

$$W = \frac{(2.3 \times 10^{-3})(N)(Pmd)(S)}{\left[\frac{Pmd}{909.1}\right]^{0.78}} =$$

EXPOSURE:

Normal: ______________ mg/m^3

Worst Case: ______________ mg/m^3 (6 times normal case)

No. of Workers: _________

Figure 4. Manufacturing exposure worksheet.

PLANT VICINITY POPULATION EXPOSURE

CHEMICAL: ______________________________ NO. __________

Maximum Daily Production, Pmd, ____________________ kg/day

$\bar{X}i$ = chemical concentration, mg/m^3 Number of Plants _____

X = distance from source, km

Pmd= maximum production, kg/day

$\bar{X}i = (1.04 \times 10^{-5})(\text{Pmd})$ for 1 km

X km	Factor	Conc. mg/m^3	Population Exposed per Plant	TOTAL
1	1.04×10^{-5}		3,660	
2	3.11×10^{-6}		14,600	
3	1.53×10^{-6}		32,900	
5	6.32×10^{-7}		91,400	
10	1.89×10^{-7}		365,700	
20	5.66×10^{-8}		1,462,700	

Figure 5. Plant vicinity population exposure worksheet.

PROCESSING EXPOSURE

CHEMICAL: ______________________________ NO. __________

Use: ______________________________

Annual Production, P, ______________________ kg/yr

Number of Plants, N, ______________________

Number of Days in Production ______________________

Number of Process Steps ______________________

Persistence, R, Gas = 1.0 Nonvolatile = 3.0

Fraction of Chemical in Product, F, ______________

Maximum Daily Production, Pmd ______________ kg/day/plant

Maximum Daily Use, (Fx) (Pmd) = A______________ kg/day

In-Plant Concentration, normal operations, Cn =

$$Cn = \frac{(4.167)(R)(A)}{(4.67)(A)+5660} = \qquad \text{mg/m}^3$$

Number of Workers Exposed, W

$$W = \frac{(2.3 \times 10^{-3})(N)(R)(Pmd)}{\left[\frac{Pmd}{909.1}\right]^{0.78}}(S) = \underline{\qquad\qquad}$$

Exposure:

Normal: ______________ mg/m³

Worst Case: ______________ mg/m³ (6X normal)

No. of Workers: ______________

Figure 6. Processing exposure worksheet.

MANUFACTURING EXPOSURE

CHEMICAL: TRIS (2,3 dibromopropyl phosphate) NO. 1

Annual Production, P, 4.07×10^6 kg/yr

Number of Plants, N, 1

Number of Days in Production, D, 360

Number of Process Steps, S, 3

Persistence, R, Gas = 1.0 Nonvolatile = 3.0

Maximum Daily Production Pmd 11,300 kg/day

In-Plant Concentration, normal operations, Cn =

$$Cn = \frac{(4.167)(R)(Pmd)}{(4.67)(Pmd)+5660} = \frac{(4.167)(1)(11,300)}{(4.67)(11,300)+2830} = 8.8\ \text{mg/m}^3$$

Number of workers exposed, W,

$$W = \frac{(2.3 \times 10^{-3})(N)(Pmd)(S)}{\left[\frac{Pmd}{909.1}\right]^{0.78}} = \frac{(2.3 \times 10^{-3})(1)(11,300)(3)}{\left[\frac{11,300}{909.1}\right]^{.78}} = 11$$

EXPOSURE:

Normal: 0.8 mg/m³

Worst Case: 4.8 mg/m³ (6x)

No. of Workers: 11

Figure 7. Manufacturing exposure, TRIS.

PLANT VICINITY POPULATION EXPOSURE

CHEMICAL: TRIS (2,3 dibromopropyl phosphate) NO. 1

Maximum Daily Production, Pmd, 11,300 kg/day

$\bar{X}i$ = chemical concentration, mg/m³

X = distance from source, km

Pmd= maximum production, kg/day

$\bar{X}i = (1.04 \times 10^{-5})(Pmd)$ for 1 km

X km	Factor	Conc. mg/m	Population Exposed
1	1.04×10^{-5}	0.117	3,660
2	3.11×10^{-6}	0.035	14,600
3	1.53×10^{-6}	0.017	32,900
5	6.32×10^{-7}	0.0071	91,400
10	1.89×10^{-7}	0.00213	365,700
20	5.66×10^{-8}	0.00064	1,462,700

Figure 8. Plant vicinity population exposure, TRIS manufacture.

PROCESSING EXPOSURE

CHEMICAL: TRIS (2,3 dibromopropyl phosphate) NO. 1

Use: Carpet Manufacture

Annual Production, P, 2.95×10^7 kg/yr

Number of Plants, N, 10

Number of Days in Production 360

Number of Process Steps 5

Persistence, R, Gas = 1.0 Nonvolatile = 3.0

Fraction of Chemical in Product, F, 0.10

Maximum Daily Production, Pmd 8,000 kg/day/plant

Maximum Daily Use, Fx Pmd = A 800 kg/day

In-Plant Concentration, normal operations, Cn =

$$Cn = \frac{(4.167)(R)(A)}{(4.67)(A)+5660} = \frac{(4.156)\ (3)\ (800)}{(4.67)\ (800) \div 5660} = 1.06 \text{ mg/m}^3$$

Number of Workers Exposed, W

$$W = \frac{(2.3 \times 10^{-3})(N)(\text{PMD})(S)}{\left[\frac{\text{PMD}}{909.1}\right]^{0.78}} = \frac{(2.3 \times 10^{-3})\ (10)\ (8000)\ (5)}{\frac{8000}{909.1}\ .78} = 169$$

Exposure:

Normal: 1.0 mg/m^3

Worst Case: 6.0 mg/m^3

No. of Workers: 169

Figure 9. Processing exposure, carpet manufacture, TRIS.

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SECTION 4

PREDICTION OF EXPOSURE DURING CONSUMER USE

While some new chemicals will lose their identity during processing, others will be used by the general public, either as produced or as an essential component of a formulation. Thus it was necessary to specify and document procedures for rapid estimation of the chemical dose (mg/person) and the population receiving that dose (person) due to the use of consumer products. Dose is defined to be the amount of a chemical that enters the human body. Exposure is the amount of chemical in proximity to the human body in a form such that it has substantial probability of becoming dose.

People receive chemical dose from consumer products via oral, inhalation and skin contact routes. Though in a given case, any one of these routes may be dominant, generally speaking, the oral route is most significant, then inhalation, then skin contact. Statistics compiled by the National Center for Health Statistics (NCHS) suggest that at least 1,200 people yearly receive oral doses of between 5 and 30 grams of single chemicals in paints, cleaning agents, disinfectants and petroleum products, based on the number of fatalities and the corresponding toxicities (Gleason 1969). Inhalation doses can also be in the range of grams per year. Since a person breathes about one cubic meter of air per hour when active (Handy 1974), a chemical with a molecular weight of about 100, present at one part per thousand, would result in an inhalation of about 5 grams per hour, not all of which would become dose. For carbon monoxide, the LCLo dose (lowest published lethal concentration) is 4000 ppm for 30 minutes (Fairchild 1977), which is about 2.6 g of breathed CO. Based on NCHS statistics, at least 1,100 people per year are exposed to CO at these levels, including exposure resulting from motor vehicle exhaust. Consideration of odor thresholds (Dravniaks 1976) also suggests that inhalation dose from volatile chemicals often reaches levels of grams per person. Skin contact dose is generally smaller, usually milligrams per person or less. Even though carbon tetrachloride has a mean oral lethal dose of 5 to 10 g, it is not associated with acute contact lethality. However, for aniline (mean lethal oral dose 15 to 30 g (Gleason 1969)) there have been many deaths due to skin contact: canvas shoes (Miner 1919), laundry markers and oral dose (Greenberg 1964). Iodine has caused contact poisoning death when more than one third of a person's body was painted with it (Gleason 1969).

Method and Rationale

Clearly one should be able to estimate the amount chemical dose resulting from exposure to consumer products by considering the form of the products, the characteristics of the chemicals they contain and the way they are used.

Products like polishes, waxes and paints, which involve skin contact with liquids, obviously represent a greater potential for dose than do chemicals immobilized in, say, appliance coatings or building materials. Similarly, volatile materials used indoors constitute a greater potential for inhalation dose than they would if they were used outside. Products may also involve oral contact (silverware, utensil finishes, pottery finishes, etc.).

Because of the variety of routes and exposure patterns that are involved in the use of consumer products--any one of which may be dominant in a given case--many variables would be required to characterize consumer dose at an engineering level of description. Some exposure evaluation schemes (TSCA 1978, Stalder 1979) have sidestepped the details of an engineering evaluation by scoring various component variables (duration of contact, degree of contact, volatility of component, etc.) and computing an overall score roughly representative of dose. These measures reflected only a "low resolution" estimate of dose, and are difficult to factor into a quantitative risk assessment. A recent exposure evaluation equation (Becker 1978, 1979) had more of an engineering orientation, but it did not contain sufficient variables (some were scored) and it could not be used to compute disposal masses or material balance. In an effort to address these needs (more accurate dose levels, disposal mass estimate and material balance) an engineering approach using some 34 variables, was chosen to predict consumer exposure. Of the 34 variables, about 20 characterize products and the ways they are used. Estimated values of these variables are cataloged on Table 5 for major classes of products. Twelve of the other 14 variables are obtained from the results of estimation of Physical-Chemical Parameters and Use Classes and 2 are obtained from estimation of production.

Parameters

All of the variables used to estimate consumer exposure are listed in Table 6. Of those variables, the ones relating to chemical-physical-use include: C, D, Dens, F, FNC, MW, Pi, Pv, Sol, Tres, U and Use. Of these, C, Dens, FNC, MW, Pi, Pv, U and Use are discussed in depth in Sections 5 and 6 of this report. D, the diffusivity, expresses the ability of the chemical, C, to escape from the product, as compared to its escape from the pure chemical. For example, a volatile pigment would volatilize in a given amount of time, as a pure substance. However, when combined with a textile, it may volatilize more slowly--or not at all--depending on the strength of its bond to the textile. D equal zero corresponds to no release, and D equal 1 corresponds to volatilization equal to that of the pure chemical.

The parameter F represents the fraction of products in a use class that contain a given chemical function category, FNC, e.g. what fraction of clothing contains flame retardant? The parameter Tres represents the time for which C would be stable in the air following volatilization. Values of Tres less than 1 hour are significant. If Tres is greater than 1 hour, the effective residence time is limited by ventilation rates. The marketing parameters used include f and Ship.

TABLE 5. CONSUMER USE CATEGORIES

		Pa	Pp	Ta (hr)	Tp (hr)	Vola (m^3)	Volp (m^3)	Sa	Sp	Sbp	Da (min)	Dp (min)	FLa	FLp	Ymin (min)	Ma	Mp	Aa (m^2)	Ap (m^2)
110	*Structural Components	0.15	1.0	6.0	-	400	400	0.05	0.10	0.0	20	5	1	0.01	10.0	0.2	0.01	0.1	0.1
113	*Caulk + Speckle	0.15	1.0	4.0	-	400	400	0.05	0.15	0.0	20	5	1	0.01	5.0	1.0	0.01	0.1	0.1
115	Brick	0.02	1.0	5.0	10^5	400	400	0.03	0.03	0.0	10	5	1	0.01	10.0	0.03	0.01	0.1	0.1
116	Wood	0.05	1.0	5.0	10^5	400	400	0.05	0.03	0.0	10	5	1	0.01	5.0	0.03	0.01	0.1	0.1
117	Concrete	0.1	1.0	10.0	10^5	400	400	0.05	0.03	0.0	20	10	1	0.01	10.0	0.3	0.01	0.1	0.1
120	*Paint - All	0.15	1.0	24.0	10^5	100	100	0.05	0.30	0.0	10^3	10	1	0.03	1.0	1.0	0.01	0.1	0.1
121	*Paint Exterior and Materials	0.15	1.0	24.0	10^5	400	400	0.02	0.50	0.0	10^3	10	1	0.01	1.0	1.0	0.01	0.1	0.01
122	*Paint Interior; Wallpaper and Materials	0.15	1.0	24.0	10^5	40	40	0.02	0.05	0.0	10^3	10	1	0.05	1.0	1.0	0.01	0.2	0.1
124	Floor; Furniture and Shoe Wax	0.60	1.0	24.0	10^5	40	40	0.05	1.0	0.05	750	100	1	0.05	0.2	1.0	0.01	0.2	0.1
130	Furniture	0.0	1.0	0.0	10^5	0	40	0.0	0.01	0.0	0	10^3	0	0.1	5.0	0.0	0.02	0.0	0.2
140	Plumbing + Supplies	0.1	1.0	24.0	10^3	40	40	0.03	0.01	0.0	10^3	10^3	1	0.01	2.0	2.0	0.01	0.2	0.1
141	*Water Softening and Other Treatment	0.4	0.5	12	-	40	40	0.01	0.01	0.0	10^5	10^5	1	0.01	2.0	2.0	0.01	0.1	0.2
144	*Sanitizer - Cleaner	0.50	1.0	25	-	40	40	0.02	0.01	0.95	100	200	1	0.01	0.1	1.0	1.0	0.02	1.0
146	*Corrosion Treatment	0.15	0.5	0.2	-	40	40	0.05	0.01	0.0	10	30	1	0.01	0.1	1.0	0.5	0.02	0.1
150	Heating; Cooling	0.05	1.0	0.5	2	40	40	0.001	0.001	0.0	1	0	1	0.01	0.0	1.0	1.0	0.02	0.0
151	Oven Cleaners	0.1	0.5	10	10^4	40	40	0.03	0.03	0.98	1	0	1	0.03	1.0	1.0	1.0	0.01	0.0
160	Eating	1.0	0.1	10^2	10^4	40	40	0.01	0.01	0.0	50	50	1	0.2	2.0	0.01	0.01	0.1	0.1
172	*Metal Polish	0.15	1.0	12	-	40	40	0.02	0.005	0.99	500	500	1	0.05	0.05	1.0	1.0	0.1	0.1
173	*Deodorizer	0.30	1.0	20	100	40	40	1.0	0.0	0.0	10	0	1	0.0	-	1.0	1.0	0.1	0.1
175	Fire Extinguishers	0.1	0.1	2	1	40	40	0.95	0.0	0.05	5	0	1	0.3	3.0	1.0	1.0	0.2	0.2
200	Clothing (additives)	0.0	1.0	0	$2.5x10^5$	40	40	0	0.05	0.05	0	10^4	0	0.3	0.05	0.0	0.05	1.0	1.0
210	Fabric	0.0	1.0	0	10^4	0	40	0	0.05	0.05	0	10^5	0	0.3	1.0	0.0	0.05	0.0	1.0
220	Jewelry	0.0	1.0	0	10^3	0	40	0	0.01	0.0	0	10^4	0	0.1	1.0	0.0	0.01	0.0	0.05
233	*Cleaners; Detergents Soaps; etc.	1.0	1.0	100	-	40	40	0.05	1.0	0.98	3×10^3	10^3	1	0.02	1.0	1.0	1.0	0.1	2.0
236	*Bleach	0.5	1.0	0.1	-	40	40	0.02	0.0	0.99	1	10^5	1	0.01	0.1	1.0	1.0	0.0	0.0
305	Dust Control Agents	0.05	0.3	50	10^4	40	40	0.03	1.0	0.96	100	2	1	0.2	1.0	1.0	1.0	0.1	0.1
311	*Fuel	1.0	1.0	0.0	-	400	400	0.02	0.98	0.0	0	10	0	0.2	-	1.0	1.0	0.0	0.1
312	Tires	0.0	1.0	10^4	10^4	400	400	0.0	0.5	0.0	0	60	0	0.1	4.0	0.0	0.5	0.0	0.1
313	*Oil and Grease (car)	0.0	1.0	0.0	-	400	400	0.0	0.05	0.0	0	100	0	0.1	5.0	0.0	1.0	0.0	0.1
314	*Batteries	1.0	1.0	0.1	10^3	400	400	0.01	0.05	0.94	1	0	.05	0.005	5.0	1.0	1.0	0.1	0.0
315	*Antifreeze	0.20	0.20	0.1	-	400	400	0.01	0.05	0.94	3	0	1.0	0.01	5.0	1.0	1.0	0.1	0.0
410	Hair Spray	0.3	1.0	10	10^{10}	40	40	0.3	0.05	0.3	10^4	0	1.0	0.2	0.05	1.0	1.0	0.1	0.0
420	*Soap	1.0	0.0	50	10^{10}	40	40	0.30	0.02	0.95	3000	0	1.0	0.0	-	1.0	0.0	2.0	2.0
430	Body Powder - Cosmetics	1.0	1.0	8	10^{10}	40	40	0.31	0.02	0.90	500	0	1.0	0.2	0.02	1.0	1.0	0.1	0.0
440	Antiperspirants	1.0	1.0	8	10^{10}	40	40	0.2	0.2	0.6	10^5	10^4	1.0	1.0	0.01	1.0	1.0	0.2	0.0
450	Cologne	0.3	1.0	10^4	10^{10}	40	40	0.2	0.2	0.6	10^5	0	1.0	1.0	0.01	1.0	1.0	0.3	0.0
460	Suntan Lotions	0.2	0.0	100	0	400	0	0.2	0.0	1.0	$6x10^4$	0	1.0	0.0	0.05	1.0	0.0	0.6	0.0
470	Depilatories	0.2	0.0	10	0	400	0	0.2	0.0	1.0	300	0	1.0	0.0	0.05	1.0	0.0	0.3	0.0
500	*Agriculture and Gardening Chemicals	0.03	0.20	1	-	400	400	0.2	0.7	0.0	20	0	0.2	0.05	0.05	0.3	0.1	0.1	0.1
630	*Bath and Swimming Chemicals	0.001	0.5	1	100	400	400	0.02	0.90	0.08	60	$6x10^4$	1.0	0.01	-	1.0	1.0	0.1	2.0
660	*Books and Printed Materials	0.0	1.0	100	10^5	40	40	0.001	0.001	1.0	$6x10^3$	0	0.1	0.01	0.05	0.1	0.1	0.0	0.1
670	Fireworks + Explosives	0.05	0.1	2	2	400	400	0.3	0.3	0.0	5	0	1.0	0.3	3.0	0.1	1.0	0.1	0.0
680	*Crafts	0.1	1.0	100	-	40	40	0.15	0.05	0.80	$6x10^3$	0	1.0	0.1	1.0	1.0	1.0	0.1	0.1
691	*Correction Fluid	0.1	0.1	10	0	40	40	0.10	0.0	0.90	60	0	1.0	0.05	0.05	1.0	0.0	0.1	0.1
700	*Packaging Non-Food, Food	0.0	1.0	0	10^4	40	40	0.0	0.1	0.0	0	10^3	0.0	0.1	1.0	0.0	0.1	0.0	0.1
720	*Adhesives	1.0	1.0	10	-	40	40	0.05	0.0	0.95	10	20	1.0	0.05	1.0	0.5	0.1	0.1	0.1
730	*Propellents	1.0	1.0	1	1	40	40	0.95	0.0	0.05	0.95	0	0.2	0.2	-	1.0	1.0	0.2	0.2
800	*Consumer Plastic	0.0	1.0	0	10^{10}	0	40	0.01	0.05	0.0	0.0	100	0.0	1.0	5.0	0.0	0.01	0.1	0.1
801	*Consumer Rubber	0.0	1.0	0	10^{10}	0	40	0.01	0.3	0.0	0.0	100	0.0	1.0	5.0	0.0	0.3	0.1	0.1
810	*Animal + Insect Repellents	0.1	0.0	1	1	400	400	0.98	0.0	0.02	1.0	10	1.0	0.0	-	1.0	0.0	0.2	0.2

TABLE 6. VARIABLES USED TO ESTIMATE CONSUMER EXPOSURE

Symbol	Meaning	Units	Source of Evaluation
Aa	Body area in contact with product during active phase	M^2	Table 5
Ap	Body area in contact with product during passive phase	M^2	Table 5
C	Name of chemical	--	PMN
Ca	Effectiveness of skin contact with chemical-active phase	-(0-1)	Page 34
Cp	Effectiveness of skin contact with chemical-passive phase	-(0-1)	Page 34
D	Chemical Diffusivity	-(0-1)	Section 6
Da	Contact duration with product per year per person active phase	minutes	Table 5
Dens	Chemical Density	g/cc	Section 6
Dose a	Active phase chemical dose per exposed person per year	mg/(person-yr)	Page 35
Dose p	Passive phase chemical dose per exposed person per year	mg/(person-yr)	Page 35
Dp	Contact duration with product per year per person passive phase	minutes	Table 5
f	Predicted market penetration by C	-(0-1)	Section 5
F	Fraction of product in a USE class containing specific FNC	-(0-1)	Section 6
FNC	EPA chemical Function Category	--	Section 6
Fva	Fraction of chemical in product volatilized during active phase	-(0-1)	Page 36
Fvp	Fraction of chemical remaining in product volatilized during passive phase	-(0-1)	Page 36
La	Population loading active phase	-(0-1)	Table 5
Lp	Population loading passive phase	-(0-1)	Table 5
Ma	Fraction of remaining mass of C available to become dose - active phase	-(0-1)	Table 5
Mp	Fraction of remaining mass of C available to become dose - passive phase	-(0-1)	Table 5
MW	Molecular weight of C	AMU	Section 6

TABLE 6. (cont.)

Symbol	Meaning	Units	Source of Evaluation
Pa	Fraction of total population using products in a use class - active phase	-(0-1)	Table 5
Pi	Partition coefficient of C	--	Section 6
Pop(a)	Population exposed to C, active phase, due to a specific use	people	Page 35
Pop(p)	Population exposed to C, passive phase, due to a specific use	people	Page 35
Pp	Fraction of total population using products in a use class - passive phase	-(0-1)	Page 35
Pv	Vapor pressure	mm of Hg	Section 6
Sa	Fraction of C in product undergoing non-volatile release - active phase	-(0-1)	Table 5
Sbp	Fraction of C in product undergoing non-volatile release - passive bypass phase	-(0-1)	Table 5
Ship	Total Shipments in one FNC category	kg	Table A-3
Sol	Solubility of C in water	mass fraction -(0-1)	Section 6
Sp	Fraction of C remaining in product non-volatile release - passive phase	-(0-1)	Table 5
Ta	Average lifetime of product - active phase	sec	Table 5
Tp	Average lifetime of product - passive phase	sec	Table 5
Trel	Time for 50% of C to be volatilized from product	sec	Page 33
Tres	Residence time for C in respirable air	sec	Section 6
U	Fraction of C used in a specific USE class	-(0-1)	Section 6
Use	Use category	--	Section 6
Vola	Dilution volume - active phase	m^3	Table 5
Volp	Dilution volume - passive phase	m^3	Table 5
Y	Thickness of the chemical layer in the product	mm	Table 5

The market penetration parameter, f, is generated as discussed in Section 5 and equals the fraction of a given FNC market that C would be expected to capture. Ship equals the total shipments in an FNC market, so that f ship equals the projected shipments for a new chemical due to use in one FNC market.

The parameters of product use listed on Table 6 include Aa, Ap, Ca, Cp, Da, Dp, La, Lp, Ma, Mp, Pa, Pp, Sa, Sp, Sbp, Ta, Tp, Vola, Volp, and Y.

The "population active" parameter, Pa, has a range of from 0 to 1 and equals the fraction of the total population that is involved with the "active phase" use of a product. The "active phase" term is used to distinguish the different ways in which the chemicals in a product may be encountered. For example, a house paint gives dose to the painter (active phase) and to the people who later live with the painted materials (passive). Similarly, floor polishes, furniture polishes, paint strippers, detergents, soaps, bleaches, and many other classes of consumer products result in "active phase" and "passive phase" exposure, each involving separate parameters. The population active refers to those persons exposed during the active phase. The passive population (0-1) refers to the population exposed during the passive phase.

The "population loading factors" (0-1) refer to the probability that a person is present during the relevant phase of exposure. So, for painting, the loading factor for the active phase is 1, since someone must be present to do the painting. However, the loading factor for the passive phase is estimated to be only about 0.05, indicating that, taking into account all the different kinds of painting that are done; a person is in the presence of a specific painted surface only about 5% of the time. The population loading factor is significant in that it should be roughly proportional to population dose--i.e. the population gets more dose if it has greater exposure.

The "material thickness" parameter, Y, equals the thickness (mm) of the material in which the chemical is embedded. In the case of a paint, the thickness is about 1 mm. Some fabric finishes have thickness of only 0.1 mm. Structural materials (housebrick, tile, etc.) have larger characteristic dimensions. The thickness parameter contributes to the estimate of how long it takes for volatiles to escape from the material.

The "contact" parameter characterizes the degree of contact between the product and the skin. This parameter is assigned in accord with the following examples:

Contact	Description
1	pure substance (liquid): ammonia, alcohol
% comp	substance in a matrix that does not inhibit escape: swimming pool chemicals, paint, polish and soap
% comp D	substances in a retentive matrix: clothing, handles, books, appliances, decorations

The "duration" parameters (min), Da and Dp are a measure of the amount of time that contact is maintained between the amount of the product that a person would buy in one year (active and passive phases) and the skin, during the lifetime of the product. Note that the lifetime of the product may be longer than 1 year.

Duration (min)	Product Classes
3×10^5	Clothing
1×10^4	Soap
3600	Magazine Covers
300	Furniture Wax
100	Propellants
1	Fuels, Heating System Chemicals

The "area" parameters (Aa and Ap) equal the skin area of a person that is generally involved with exposure to the chemical. For a swimming pool chemical, or for a chemical used in clothing, all of the person's area would be in contact with the product. Items like paints, polishes and books involve only smaller values. The total skin area is assumed to be $2.0\ m^3$.

The "material" parameters (0-1) (Ma and Mp) equal that fraction of the chemical available to become contact dose at some time during the product lifetime. For example, in painting, virtually all of the paint is available for dose during active painting, whereas, in plastic, some of the material is never available for dose. In general, liquids and gases have high "material" availability values, and solids have lower values.

The "mass lost" parameters (0-1) are used to account for the fraction of bulk mass of the material of a product that is present at the beginning of each phase (active-Sa, passive-Sp, passive-bypass-Sbp) but lost by the end of that phase due to non-volatile processes (spilling, abrasion, etc.). The passive bypass phase involves a disposal of material following active use - such as the disposal of polishing agents, laundering agents and cleaning agents. The idea is that during each activity, such as painting, some of the mass of the material is lost, and that by keeping track of where it is lost, one can also keep track of where the chemicals it contains are lost--a materials balance approach to consumer exposure. For painting, the mass lost parameter for the active phase is estimated to equal 0.05, meaning that about 5% of paint is released during the active phase. Similarly, the mass lost parameter for the passive bypass phase for furniture polish is estimated to be about 0.95. The non-volatile dose in the active phase is included in Sa. The volatile dose is separate.

The residence time parameter Tres, (seconds) equals the time that 50% of the volatilized chemical would survive in the air and be available for inhalation dose. Direct consumer inhalation dose is most significant for exposure within houses and enclosures where the concentration of the chemical is confined. Under those circumstances, the concentration is limited by several processes: ventilation, surface adsorption and chemical reaction. The work of Young et al 1978 suggests that the ventilation limited value for residence time is about 1 hour. In the absence of additional data, this value will be assumed to apply.

The "exposure time" parameters (Ta, Tp) (hours) characterize the amount of time that the product obtained in one year lasts to give inhalation dose in the active and passive phases. So, for example, if the active phase of painting lasts for about 8 hours (active phase exposure time), but if some volatile components are not completely volatilized for 100 hours, (Trel = 100 hours) the dose during the 8 hour period is characterized by the released material (about 8/100 of the total volatilized). Alternatively, if all the material is volatilized during the active period, then none remains to lead to dose during the passive period.

The "dilution volume" parameters (Vola and Volp) equal the average volume into which the volatile material may be expected to diffuse. For uses typically indoors, the dilution volume was chosen to be 40 cubic meters. For outdoor exposure the volume is essentially unlimited by barriers, and the degree of chemical concentration in the air is heavily dependent on the wind conditions. To simulate the diffusion limitations under still air conditions, the value of the dilution volume for outdoor exposure was chosen equal to 400 cubic meters.

The variables calculated from these parameters include: Dose (a), Dose (p), Fva, Fvp, Pop (a), Pop (p) and Trel.

As indicated earlier, Trel is the amount of time it takes for C to volatilize from a product. (If C is non-volatile, Trel is infinite.) Fva is the fraction of C that volatilizes in the active phase. In a simple case, if the active phase lasts 8 hours, and Trel is 200 hours, then Fva would be at most 0.04 (subject to competition from other routes). Fvp is defined similarly, as the fraction of C volatilizing during the passive phase.

Pop (a) and Pop (p) are the populations (persons) expected to receive a dose of C during the active and passive phases respectively. So, for example, if a new flame retardant were to come on the market and be expected to capture 10% of it, the exposed passive population would be about 6 x 10^6 people, i.e. (3 x 10^8 people using clothes) (20% of clothes contain flame retardant) (0.1 market fraction).

Dose (a) and Dose (p) are the average dose for C received by the active and passive populations, respectively. So, if 1 million people are exposed to some C and collectively internalize 100 kg of it, the average dose is 100 mg.

Calculation of Dose Per Person, Exposed Population, Release and Disposal Mass

The equations for dose per person are:

$$\begin{aligned} \text{Dose (a)} = {} & \frac{(\text{Fva} + 0.01\ \text{Sa})}{\text{Max}\ (1,\ \text{Fva} + \text{Sa})} \left| \frac{\text{Tres}}{3600\ \text{Vola}} \quad \frac{\text{La Ship}}{\text{Pa}\cdot 3\text{x}10^{2}} + \right. \\ & \text{Min} \left[\frac{0.99\ 10^{6}\ \text{Sa La Ship}}{\text{Max}\ (1,\ \text{Fva} + \text{Sa})\ \text{Pa}\cdot 3\text{x}10^{8}}, \right. \\ & \left. \text{Aa Da Ca}\sqrt{\text{Solc MW}} \cdot 10^{(4-0.6|\log\ (\text{Pi})|)} \right] \end{aligned} \tag{1}$$

$$\begin{aligned} \text{Dose (p)} = {} & \frac{(\text{Fvp} + 0.01\ \text{Sp})}{\text{Max}\ (1,\ \text{Fvp} + \text{Sp})} \left| \frac{\text{Tres}}{3600\ \text{Volp}} \right. \\ & \frac{\text{Lp Ship}\ \ \text{Max}\ [0,1-(\text{Fva} + \text{Sa})]\ (1-\text{Sbp})}{\text{Pp}\cdot 3\text{x}10^{2}} \\ & + \text{Min} \left[\frac{0.99\ \text{Sp}\ 10^{6}\ \text{Lp Ship Max}\ (0,1-(\text{Fva} + \text{Sa})(1-\text{Sbp})}{\text{Max}\ (1,\ \text{Fvp} + \text{Sp})\ \text{Pp}\cdot 3\text{x}10^{8}}, \right. \\ & \left. \text{Ap Dp Cp}\sqrt{\text{Solc MW}} \cdot 10^{(4-0.6|\log\ (\text{Pi})|)} \right] \end{aligned} \tag{2}$$

There are two equations for dose because, for many products, dose may result from different kinds of use. For example, a housepainter receives dose while painting a wall, Dose (a), while the people who live there will receive dose for many years thereafter, Dose (p), by virtue of chemicals that slowly escape from the surface.

The equations for the size of the exposed populations are:

$$\text{Pop (a)} = \text{Pa} \cdot \text{f} \cdot \text{F} \cdot 3 \times 10^{8} \tag{3}$$

$$\text{Pop (p)} = \text{Pp} \cdot \text{f} \cdot \text{F} \cdot 3 \times 10^{8} \tag{4}$$

Again, there are two exposed populations--as above, the number of people who paint, and the number of people who live near painted surfaces.

The equations for the disposal mass and the volatile and non-volatile release are:

$$\text{Rv} = \text{Ship}\cdot\text{f}\cdot\text{F} \left[\frac{\text{Fva}}{\text{Max}\ (1,\ \text{Fva+Sa})} + \frac{\text{Fvp}\ (1-\text{Sbp})\ \text{Max}\ [0,1-(\text{Fva+Sa})]}{\text{Max}\ (1,\ \text{Fvp} + \text{Sp})} \right] \tag{5}$$

$$\text{Rnv} = \text{Ship}\cdot\text{f}\cdot\text{F} \left[\frac{\text{Sa}}{\text{Max}\ (1,\ \text{Fva+Sa})} + \frac{\text{Sp}\ (1-\text{Sbp})\ \text{Max}\ (0,1-(\text{Fva+Sa}))}{\text{Max}\ (1,\ \text{Fvp} + \text{Sp})} \right] \tag{6}$$

$$\begin{aligned} \text{Disp} = {} & \text{Ship}\cdot\text{f}\cdot\text{F} \left[\text{Sbp} + (1-\text{Sbp})\ (\text{Max}\ (0,1-\text{Fvp} + \text{Sp})) \right. \\ & \left. \cdot\ \text{Max}\ (0,1-[\text{Fva} + \text{Sa}]) \right] \end{aligned} \tag{7}$$

where $Fva = \mathrm{Min}\ (Ta, Trel)/Trel$

$Fvp = \mathrm{Min}\ (Tp, Trel)/Trel$

$$Trel = \frac{4.4 \times 10^{6}\ Y\ (mm)}{D\ Pv\ (mmHg)\ MW\ (AMU)}$$

As an example of the use of these equations, consider the TRIS used in rugs.

From Section 6 we obtain:

$D = (0.0 \text{ to } 0.025)$, $Dens = 2.24$, $F = 0.8$, FNC = Flame Retardant,
$MW = 297$, $\log Pi = 7.5$, $Pv = 10^{-5}$ mm,
$Sol = 10^{-3}$ $Tres \leq 1$, $U = 0.9$, use = Rugs

From Section 5 we obtain:

$f = 0.03$, $Ship = 1.6 \times 10^{8}$

Since the use category, "rugs" is not explicitly present on Table 6 (which will often be the case) the following values were obtained by rule of thumb extrapolation from the table (X means not needed).

Aa = x, Ap = 0.1, Ca = X, Cp = 0.1, Da = X,
Dp = 5000, La = X, Lp = 0.1, Ma = X, $Mp = 10^{-3}$,
Pa = X, Pp = 0.9, Sa = X, Sbp = 0.05, Sp = 0.05,
Ta = X, $Tp = 3.6 \times 10^{8}$, Vola = X, Volp = 40

This set of assumptions leads to the following results:

$$Trel = 8.8 \times 10^{6}\ Y/(D\ P\nu\ MW) \geq \frac{(4.4 \times 10^{6})(0.1)}{(10^{-5})\ (297)\ (0.025)} = 5.8 \times 10^{9} \text{ sec}$$

$$Fva = \frac{\mathrm{Min}\ (Ta, Trel)}{Trel} = X$$

$$Fvp = \frac{\mathrm{Min}\ (Tp, Trel)}{Trel} \leq \frac{3.6 \times 10^{8}}{5.8 \times 10^{9}} = \sim 0.06$$

$$Pop\ (a) = Pa \cdot f \cdot F \cdot 3 \times 10^{8} = X$$

$$Pop\ (p) = Pp \cdot f \cdot F \cdot 3 \times 10^{8} = (0.9)(0.03)(0.8)(3 \times 10^{8}) = 6.4 \times 10^{6}$$

Dose (a) = X

$$\text{Dose (p)} = \frac{10^6[(0.06) + (0.01)(0.05)}{\text{Max }(1,\ 0.06 + 0.05)} \ \frac{3600}{3600\ 40} \ \frac{(0.1)\ (1.6 \times 10^8)}{(0.9)\ (3 \times 10^8)} \cdot$$

$$\text{Max }(0,1-[0.06 + 0.05])(1-0.05) +$$

$$\text{Min}\left[\frac{(0.99)\ 10^6\ (0.05)(0.2)(1.6 \times 10^8)\ \text{Max }(0,1-(0.06 + 0.05))(1-0.05)}{\text{Max }(1,\ 0.06 + 0.05)(0.9)(3 \times 10^8)},\right.$$

$$\left.(0.1)(5 \times 10^3)(0.1)\cdot\sqrt{10^{-3}\cdot 297}\cdot 10^{(4-0.6|7.5|)}\right]$$

$$\text{Dose (p)} = 7.5 + 8.0 \simeq 16 \text{ mg}$$

$$Rv = (1.6 \times 10^8)(0.03)(0.9)[0 + \frac{0.06}{1}(1 - 0.05)(1)] \simeq 2.2 \times 10^5 \text{ kg}$$

$$Rnv = (1.6\times10^8)(0.03)(0.9)[0 + \frac{(0.05)(0.95)}{\text{Max}(1,\ 0.11)}\text{ Max }(0,1)] \simeq 2.0 \times 10^5 \text{ kg}$$

$$\text{Disposal} = (1.6 \times 10^8)(0.03)(0.9)[(0.05) + (0.95)(\text{Max } 0,\ 0.89)]\text{Max }(0,1)$$

$$\simeq 3.8 \times 10^6 \text{ kg}$$

Discussion of Example--

Although the vapor pressure of TRIS is very low, rugs have such a long lifetime in the home that it is conceivable that some appreciable fraction of it could vaporize. Because it takes about 40 machine launderings to remove most TRIS from pajamas, the bond between TRIS and fiber must be fairly strong --leading to the estimate that the diffusivity lies in the range between 0 and 0.025. If the diffusivity were as high as 1, the expected Trel would have been 2.9 x 10^8, so that most of it would have been volatilized during its lifetime in spite of the low vapor pressure. However, using the upper bound value for D of 0.025 leads to a prediction that only 6% is volatilized. The prediction that market penetration would be 3% and that 90% of that would be used on rugs leads to the estimate that 4.3 x 10^6 kg would be used on rugs each year and that 6.4 million people would be exposed to it. Since the TRIS would be professionally applied to the carpet, there would be no active phase consumer dose. The dose equation predicts a per person dose of about 0.16 mg. The volatile release is about 2.2 x 10^5 kg, non-volatile release is 2.0 x 10^5 kg and the amount of Tris destined for disposal is 3.8 x 10^6 kg. The 16 mg would be taken up over a period of perhaps 20 years, for a rate of about 0.8 mg per year. Because of the uncertainties involved, this estimate may be in error by several orders of magnitude. However, it does focus attention on the critical parameters and indicates the problable dose range.

Engineering Details

Conceptually, analysis begins with the active phase dose. During the active phase, a volatile chemical may become dose (or release) by either a volatile or a non-volatile route (contact). The procedure used to account for this competition of routes is to calculate "rates" for each one separately, as if each route had sole access to all of the chemical, and then to apportion chemical to each route based on the calculated rates. The first step is to calculate the release volatile time. This is done by using the equation:

$$\text{Trel (sec.)} = \frac{4.4 \times 10^6\ Y\ D}{Pv\ MW} \qquad (10)$$

where D = diffusivity (0-1)

Y = thickness of the material layer (mm)

Pv = the vapor pressure of the chemical (mm Hg)

MW = the molecular weight of the chemical (AMU)

The derivation for this equation is given in the Appendix, and is based on the following argument. In a static system, the vapor released by the volatilizing material is in equilibrium with the material condensing out of the air. In that circumstance, the rate of re-entry of material (which equals the outflow) can be calculated in terms of the vapor pressure. Then, under non-equilibrium conditions, the rate of volatilization can be calculated by using this rate in a solution of the one-dimensional diffusion equation.

After the release volatilization time has been calculated, the initial estimate for the fraction of the chemical that undergoes volatile release in the active phase can be calculated via the equation:

$$\text{Fva} = (\text{Min}\ [\text{Ta}, \text{Trel}]/\text{Trel})$$

This estimate will be good unless competition with non-volatile release is severe. The corresponding estimate for the fraction of non-volatile chemical release during the active phase is Sa, a scored parameter. So, taking the competition into account, the revised estimates are:

$$\text{Fva}' = \frac{\text{Fva}}{\text{Max}\ (1,\ \text{Fva} + \text{Sa})} \qquad (11)$$

$$\text{Sa}' = \frac{\text{Sa}}{\text{Max}\ (1,\ \text{Fva} + \text{Sa})} \qquad (12)$$

The volatilized material that results in direct inhalation dose during the active phase is then given (mg) by:

$$\text{Inhalation Dose Active Direct} = \frac{10^6\ \text{Fva}'\ \text{Tres}}{3600\ \text{Vola}}\ \frac{\text{La Ship}}{\text{Pa.}\ 3\text{x}10^8} \qquad (13)$$

The basis for this equation is the following. Suppose that a vapor is released into a closed room. Suppose that the vapor will remain in the room for only one hour, and that after that it will either be swept out, be ventilated or it will chemically decompose. Suppose that a person is in that room and that during the one hour that the chemical is there, he will breathe 1 cubic meter of air (Handy 1974). Then, the amount of vapor that he will breathe during the 1 hour is:

Vapor breathed = (Vapor present)(1 cubic meter/room volume)

The loading factor should also be present in equation because the volatile material leads to dose only when a person is present. Actually, for total dose, it makes no difference over what time schedule the volatile is released. No matter what rate it is released at, on the average, any concentration will persist for 1 hour and will be subject to the same probability of being inhaled. If, however, the release time is longer than the product lifetime, then the volatile will exit via the disposal stream. This will occur for some highly volatile materials with short use times (cleaning fluids) and for many low volatility materials present in products of intermediate use times (flame retardants in clothes). Note that all inhaled material is treated as dose. A less conservative model would also account for material exhaled.

Similarly, using Sa' the amount of non-volatile chemical released in the active phase may be calculated as:

$$\text{Non-Volatile Active Phase} = Sa'\ La\ Ship\ f\ F$$
$$\text{availability of } C$$

Some of this material results in contact dose, some in aerosol inhalation and the rest in release. The aerosol inhalation dose could, in principle, be calculated by the methods presented above. However, the results would depend strongly on the particle size distribution and morphology. In special cases (e.g. asbestos) this data may be available to allow the effective residence time to be calculated. In the absence of additional data, 1% of the available non-volatiles are added to the volatilized fraction of chemical leading to inhalation dose, to account for the aerosols. The 1% figure is intended to account for the settling time of heavier particles. With this addition, the active inhalation dose per exposed person becomes:

$$10^6\ (Fva' + 0.01\ Sa')\ La\ Ship\ Tres/\ (3600\ Vola\ Pa\ 3\text{x}10^8 \quad (14)$$

Then, the contact dose is given by:

$$\text{Contact-Dose-Active-Direct} = Aa\ Da\ Ca\ 10^{(4-0.6|\mathrm{Log}(Pi)|)}\sqrt{Sol_c MWc} \quad (15)$$

for Dose $<< Ma\ \frac{Ship}{Pa}$

The derivation for the contact dose active direct equation is given in the Appendix, and it is based on the following arguments. The standard equation for diffusion from a region of high concentration, through a membrane, to a region of negligible concentration is:

$$\text{Permeability} = \text{mass}/(\text{area time concentration})$$

when the flow is controlled by Fick's law. More detailed discussion of pore size phenomena and other mechanisms are discussed in Section 6. Under these conditions, the permeability is a constant for a given membrane and a given chemical. That is, the ratio of the amount of mass diffusing through the membrane in a given period of time to the product of the area of the membrane with the time period and the external concentration of the chemical is a constant. Treherne (1956) (among others) determined permeability constants for various chemicals and related them to the corresponding partition coefficients. Other workers have related them to molecular weight and water solubility as well. Using these relations, one can estimate the permeability of skin for a given chemical. Then, one must express the chemical concentration in terms of product parameters. For products of high diffusivity, estimation is more difficult. If the surface material is removed as dose, additional material may not diffuse out from the interior. In that case, the surface concentration falls to a low value and dose delivery stops. To account for that case, the restriction is imposed that:

$$\text{Dose Mass} < \text{Ma Mass}$$

in other words, that the dose is less than the mass available to become dose (the dose may approach Ma Mass as an upper limit).

Next, subtract the amount of material lost during the active phase and calculate the material lost during passive-bypass by using the equation:

$$\text{Passive-Bypass Material} = \text{Sbp (Mass Remaining)} \qquad (16)$$

Then subtract the material lost due to passive-bypass; the calculations are essentially repeated for the passive phase. Using equation (11) the volatiles released during the passive phase are calculated via:

$$\text{Release Vol Passive} = \text{(Mass Remaining)}\ \frac{\text{Min (Tp, Trel)}}{\text{Trel}} \qquad (17)$$

and the associated doses are:

$$\text{Inhalation Dose Passive Direct} = 10^6\ (\text{Fvp}' + 0.01\ \text{Sp}')\ \text{La}\ \frac{\text{Tres}}{3600\ \text{Volp}} \cdot \frac{\text{Ship Max }(0,1-[\text{Fva} + \text{Sa}])(1-\text{Sbp})}{\text{Pp }.3\text{x}10^6} \qquad (18)$$

$$\begin{array}{l}\text{Contact Dose}\\ \text{Passive Direct}\end{array} = \text{Min}\ \frac{0.99\ 10^6\ \text{Sp}'\ \text{Ma Lp Ship (Max }[0,1-(\text{Fva} + \text{Sa})])(1-\text{Sbp})}{\text{Pp }.3\text{x}10^6},$$

$$\text{Ap Dp Cp}\ \sqrt{\text{Solc MWc}}\ 10^{(4-0.6|\log(\text{Pi})|)}$$

Then, the mass remaining is added to the total for disposal.

Finally, the dose distribution is calculated for cases where several overlapping populations are exposed to the same chemical by the use of several different products. To do this, it is assumed that the use of each product type is independent (i.e. that use of one product type does not affect the probability of also using another product type--for example, using housepaint does not affect the probability of also using dog repellent). Other assumptions could be used where warranted. The calculation proceeds by identifying the various distinct subpopulations (i.e. how may people use J1 and J2). Each such population is estimated via:

$$\text{Population fraction (J1 and J2)} = (Pj1)(Pj2) \qquad (20)$$

That is, the probability of using J1 and J2 equals the product of the fraction of the people using each one alone. The dose that this population gets equals the sum of the doses from J1 and J2. This procedure must be repeated for each of the possible subpopulations, which increase in number as 2 to the Nth power, where N is the number of separate contributing product classes.

COMPUTER METHODS

The procedures for exposure calculation defined in this report can be efficiently implemented as an interactive computer program. Some of the data would be entered at an interactive terminal while the rest of it would be read from data files. Because much of the data is merely to be copied from tables, use of a program would greatly speed up the data transfer process, and reduce the possibility of errors. Naturally, once the steps have been completed, the computation steps could also be done by the computer program.

Because the final task of this project was to evaluate a significant number of commercial chemicals for exposure "as if they were new chemicals," a computer program having many of the characteristics listed above was written to facilitate the process. This program, called "EXPOSE," is a prototype program, in that it lacks the efficiency and convenience a polished program; nevertheless, it does query the user for the data that it requires and it does do all of the calculations required. The program, which is in the computer language BASIC, was run on a PDP 11/34 computer running under the operating system RSX11M.

LIMITATIONS

The consumer exposure model was designed to serve as a rough screen predictor of probable consumer chemical dose obtained from the use of products containing new chemicals. Via a combination of estimation and computation procedures, it yields predictions of the desired parameters in a uniform and documentable manner for all chemicals. However, additional development work would be desirable to refine a number of features in the model to reduce uncertainty in the predictions. The highest priority features for refinement are: chemical diffusivity within a product, size and mass distributions of typical aerosols, rules for prediction of capture efficiency by the lungs, direct dose that results from unusual circumstances (fire, accidental ingestion, etc.) and estimated values of product use parameters. If these limitations are overcome, the model may contribute to dose evaluation analysis at a very refined level.

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SECTION 5

METHODS OF PREDICTING PRODUCTION VOLUME

The Premanufacture Notice (PMN) forms as proposed in the Federal Register January 10, 1979 required the applicant to state the anticipated production volume for the first year and the predicted volume of the third and fifth year. Modifications and simplification of these forms may result from the hearings and it would be desirable for the OTS to have a technique to independly predict the production growth rate of the new chemical.

Estimation of the exposure during manufacturing and during consumer use is based upon production volume and this becomes an important basic parameter for exposure assessment.

A system to predict production volume has been developed. The system utilizes the function and use categories for consumer products along with data as to the total production and number of competitors.

OBJECTIVE AND SCOPE

The objective of this task was to develop a procedure and a supporting data base to estimate the market share which a new chemical has the potential of capturing. The production volume is thus estimated for the first, third, and fifth years following market introduction. This can then be applied to estimated values of production volume as listed in Table A-1, to obtain market share by volume for first, third, and fifth year penetration. (A list of references used for many of the production volume estimates is presented at the end of Table A-1.) The chemical industry, according to U.S. Industrial Outlook and other sources, appears to experience annual volume growth ranging from 3-10%, depending on the particular chemical function category. In summary, the market share estimates which will result from the procedure are multiplied by the appropriate annual production volume figures and by an overall growth estimate of 3-10% (based on the judgement of the evaluator) to obtain one, three, and five year estimates of production volume for a new chemical.

It must be recognized at the outset that this procedure is intended as a preliminary, gross screening mechanism, and is in no way intended to represent a definitive or highly precise means of modeling the chemical marketplace or in predicting market share. The limits of this procedure are characterized in a later section in order for the user or other interested parties to understand the degree to which it represents a tentative means of estimating potential market share and production volume for new chemical products. Determination of market share for industrial market research purposes is a difficult task and typically requires a considerable level of effort in time and dollars to confidently and reliably analyze a market.

The procedure presented here identifies many of the key determining factors for a new product's market share estimation, and represents a means for estimating within an order of magnitude the likely market share, hence the production demand, for the new chemical. The procedure for estimating market share of a new chemical in specific chemical categories (i.e., markets) and the base of data needed to apply this procedure are discussed below.

PROCEDURE

The procedure for estimation of production volume is dependent upon the identification of appropriate chemical function categories as predicted on the basis of structure and/or information in the PMN forms. The procedure is applied to each identified function category in order to develop a list of the appropriate categories and corresponding market share estimates for each, for the first, third, and fifth years following introduction. Market share estimates are based on factors specific to each chemical category and on factors specific to each firm planning to introduce a new chemical. As a result market share estimates, and hence production demand estimates, cannot be stated explicitly for each category without some information about the firm itself in relation to the expected competition. These issues are discussed in the paragraphs which follow.

Five Year Market Share Estimation

The procedure begins with an estimate of the market share for the fifth year following introduction, rather than the first or third years. This is done since the fifth year value more nearly represents the total potential of a product in relation to its applications under "equilibrium" competitive market conditions. Following estimation of the fifth year potential share, the first and third year shares can be estimated based on reasonable assumptions about the market share growth for a new product.

We have developed a parametric approach for estimating new chemical market share (five years) which is based on a minimum of key variables which are (1) characteristic of the chemical category or (2) characteristic of the firm. The general relation and a description of the variables in provided below:

$$MS_{5nc} = abc\ MS_{bv}$$

where MS_{5nc} = fifth year market share estimate for a new chemical

MS_{bv} = "base value" estimate of market share for a new chemical

- The base value essentially represents a nominal, imaginary estimate which is an inverse function of the number of competitors in a given chemical cateogry identified for a new chemical. For example, if there are 25 firms competing in a category, then a starting point (i.e. base value) for estimating market share for the new chemical would be 100% ÷ 25 = 4% (0.04) market share for each firm. This represents an initial inference of no concentration of business, which is adjusted by assignment of a value to factor 'a' defined below.

- Data concerning the total number of competitors, needed for defining MS_{bv}, is described in the following section.

'a' ≡ Factor applied to MS_{bv} which takes into account whether the firm proposing the new chemical is a large or small in relation to the chemical industry as a whole.

- This is determined by the evaluation based on a list of chemical companies with sales of over 5 million dollars, available from the Kline Guide to the Chemical Industry, 1977.

- If a firm is large it is expected to have the potential to compete with the larger market share firms in the chemical category and thus for the 80% of the business which 20% of the firms represent in most industries (set a = 5).

- If a firm is small it is expected to have the potential to compete at a level comparable to the smaller market share firms in the chemical category and thus for 20% of the business which 80% of the firms represent (set a = 1.25).

'b' ≡ Factor applied to MS_{bv} which takes into account whether the firm is currently competing in the chemical category or not, and thus whether it has progressed along the learning curve, established distribution channels, established reputation, etc. This factor accounts for whether a new chemical would be able to capture its full potential market in about five years, based on the current involvement (or not) of the firm in the chemical category. (Set b = 1 if the firm is currently competing in the category, set b = 0.5 if it is not.) It is expected that this information would be determined based on knowledge of the firm and its premanufacture notice submittal. The values of 'b' are intended to provide a relative indication of the impact of the firm in penetrating the market with a new chemical. It is understood that study of historical data is needed to refine these estimates in order to define their absolute value.

'c' ≡ Factor applied to MS_{bv} which takes into account whether the chemical category is dynamic and rapidly changing (i.e., short product life cycle) or not, in terms of new product acceptance and propensity for change. This factor also determines whether a new chemical could achieve its full market potential in five years). Set c = 1 if the chemical category is "dynamic," set c = 0.5 if it is not. This information has been estimated by IITRI for each function category. (See Table A-2 column labeled "Function Type 'c'".) The values of 'c' are intended to provide a relative indication of the impact of the industry structure in penetrating the market with a new chemical. It is understood that study of historical data is needed to refine these estimates in order to define their absolute value.

Determination of Number of Competitors in a Chemical Category In Order to Identify for MS_{bv}

Once a chemical category is identified Table A-2 is used to determine the estimated number of competitors, N_T, is the category. The base value market share can then be selected from the table below. For example, if it is determined that a new chemical is represented by category number 015, Algicides, then the range for N_T is between 26 and 50. The value of MS_{bv} is then selected from the table below as 0.030.

TABLE 7. TOTAL NUMBER OF FIRMS COMPETING VS ESTIMATED BASE VALUE MARKET SHARE

Total Number of Firms Competing, N_T, in a Chemical Category	Base Value Market Share, MS_{bv}*
$N_T \leq 25$	0.065
$25 < N_T \leq 50$	0.030
$50 < N_T \leq 100$	0.0125
$100 < N_T$	0.005

*Percent values of market share are obtained by multiplying the fractional values indicated by 100.

- The table was developed based on the recognition, through experience in market research, that there is a greater propensity for a higher market share per firm if there are fewer firms competing. (This is then refined based on whether the firm is large or small, etc.)

- The base value market shares are segmented in the table in terms of ranges of N_T in order to not propose a continuous, deceptively accurate equation. This is done due to a relatively low confidence in identifying the actual specific number of firms in a category without conducting a research study. (The number is also subject to fluctuation over time.) We therefore choose not be make the relationship seem more accurate than the raw data permits.

- These estimates are intended to be on the conservative side, though with a relatively broad range of fluctuation possible. That is, if the table were plotted with N_T on the horizontal axis and MS_{bv} on the the vertical axis, the curve which results would be shifted to the right of what we would expect in reality. Our use of the ranges is based on mid-range values to calculate MS_{bv}, with the extreme limits representing the level of fluctuation. The second range value was developed as follows:

  - The mid-range of $25 < N_T \leq 50$ is about 38. This would represent a nominal 0.026 market share per firm (1 ÷ 38). We selected 0.030 in order to err on the conservative side.

  - The resulting fluctuation limits are calculated at each extreme. For $N_T = 26$, MS_{bv}, could be $1 \div 26 = 0.038$. For $N_T = 50$, MS_{bv} could be $1 \div 50 = 0.020$.

  - In summary, $MS_{bv} = 0.030 {}^{+0.008}_{-0.010}$. Since the confidence is low in predicting the exact N_T, we rely on the mid-range value.

In summary, to estimate the fifth year market share potential, the factors 'a', 'b', and 'c' are applied to MS based on Tables 6 and A-2. This then permits a determination of the one and three year estimates as described below.

One and Three Year Market Share Estimation

The one and three year estimates of market share are derived following the five year estimate. Most product growth histories follow the pattern illustrated in Figure 10 on the following page, assumed to be applicable for chemical function categories as well.[1-4]

One represents the case of potential market share attained within 5 years (i.e., a relatively short life cycle, dynamic product category). A second curve represents the case of potential market share attained within about 10 years (i.e., a relatively long life cycle, stable purchase patterns, mature product category).

The procedure for estimating one and three year market share is based on applying the following relationships:

$$MS_{1nc} = d\ MS_{5nc}$$

and

$$MS_{3nc} = e\ MS_{5nc}$$

where: MS_{1nc} = first year market share estimate for a new chemical

MS_{3nc} = third year market share estimate for a new chemical

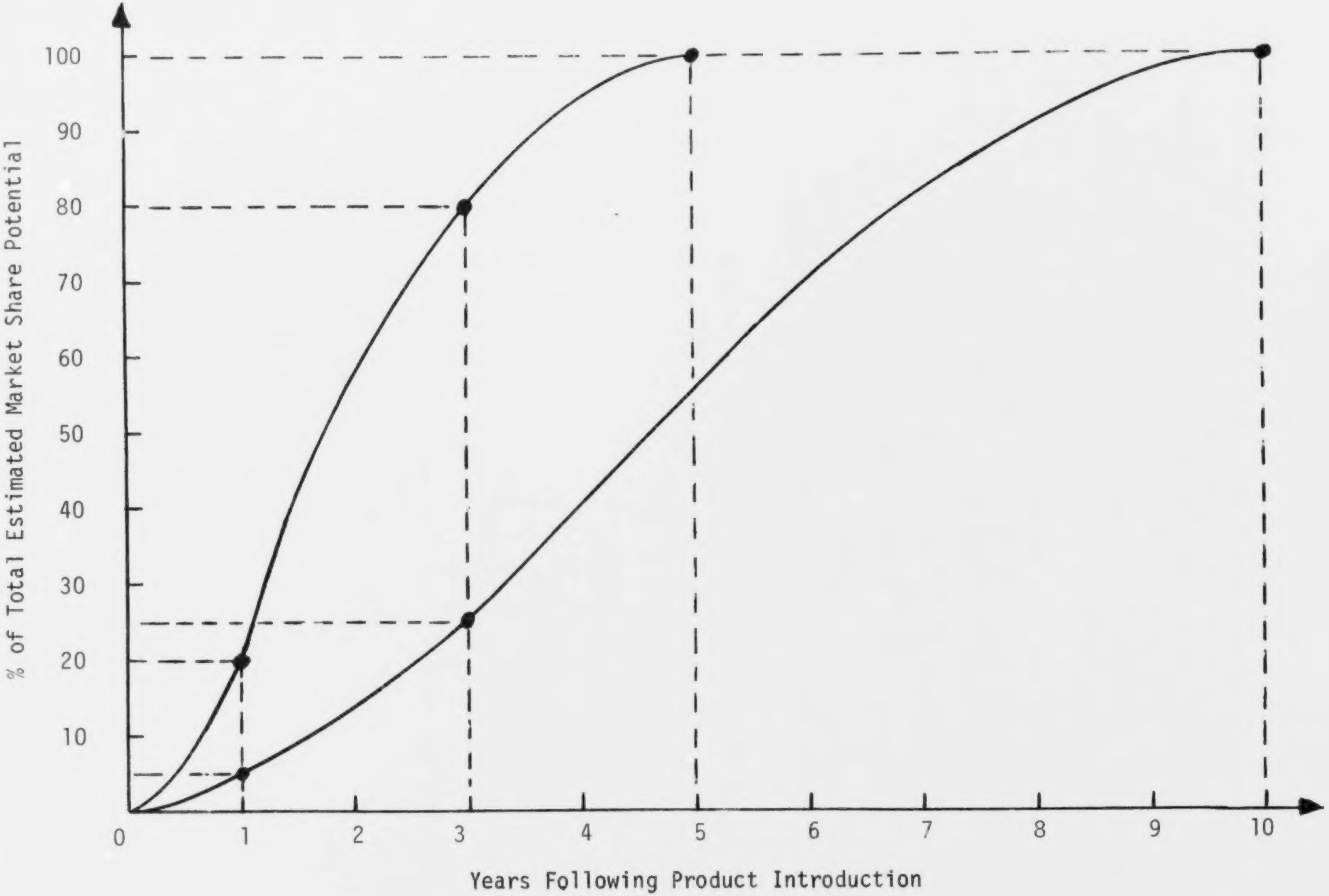

Figure 10. Idealized new product market growth for five year and ten year product growth cycles.

MS_{5nc} ≡ fifth year market share estimate for a new chemical

d ≡ factor which indicates the proportion of market share attainable after one year. (Set $d = 0.2$ for a chemical category which is identified as $c = 1$. Set $d = 0.05$ for for a chemical category which is identified as $c = 0.5$.)

e ≡ factor which indicates the proportion of market share attainable after three years. (Set $e = 0.8$ for a chemical category which is identified as $c = 1$. Set $e = 0.25$ for a chemical category which is identified as $c = 0.5$.)

Applying the variables to the two equations will yield estimates of the magnitude of the market share which could be attained after one and three years respectively, given the estimate of market share for the fifth year. (Refer to the example at the end of this section.)

ASSUMPTIONS AND QUALIFICATIONS

The following list of assumptions and qualifications is provided to assure a clear understanding of the limits of this market share estimation procedure, and the basis for its representation as a preliminary gross screening mechanism.

a) Firm may have an extensive product line, all in the same markets, and therefore the new chemical will only represent a fraction of its total business in those markets. Thus the market share estimate may be higher than would in reality exist, by assuming that a firm only offers one product in a given category. (This can be clarified in some cases by reviewing chemical catalogs, discussion with the firm, or referring to U.S. ITC reports, Thomas Register, etc.)

b) Different products of the same function may be specially tailored to distinct applications and/or user markets. Thus the market share estimate may be higher than would in reality exist, by assuming that a firm offers its product across all applications and market segments.

c) The new chemical may only represent a one time batch quantity in which case no planned, massive investment is specifically anticipated and therefore no rational market share projections are meaningful. A cursory review of the chemical advertising literature can provide an indication of the extent to which batch quantities are represented in the market place.

d) It is likely that most of the commercialized innovations, hence, the new chemicals will come from the major chemical firms (e.g. annual sales greater than 5 million dollars) in a chemical category. This is based on research of trends in innovation by leading universities, and the indication that costs of regulatory compliance will impact on the ability of small business to commercialize innovations.

e) Most new chemicals are extensions, modifications of a firm's existing product line.

f) It is less likely that a new commodity-type chemical will be introduced than a specialty chemical, due to the greater commitment required for large volume production capabilities and lesser degree of innvoation in commodity chemicals than specialty chemicals.

g) It is assumed that about 20% of the firms competing in any category will represent 80% of the business in that category. This is based on historical market indications to this effect gained in numerous market research projects over many years. Refer also to the 1972 U.S. Census of Manufactures, Concentration Ratios in Manufacturing.

h) A primary determinant in estimating market share potential is the number of firms competing in the chemical category. In fact it is estimated that long term penetration varies inversely to the number of firms competing for a product having similar cost, performance and service attributes, (i.e., a breakthrough which will capture all of the market is the exception rather than the rule.)

i) Concomitant with the previous point is the importance of the size of the firm (offering the new chemical) on its potential impact (i.e., market share or penetration) within a chemical category. A large firm is likely to beget a larger market share than a small firm due to 1) resources for regulatory compliance and R&D, and 2) innovation capacity, and 3) resources for production, promotion, distribution, etc.
Thus a firm which is large has a greater potential, hence likelihood, for being one of the 20% of the firms with 80% of the business rather than one of the 80% of the firms with 20% of the business.

j) Commodity-type is defined as a fairly standardized, high-volume chemical, whereas a specialty is a high performance, market-volatile, relatively low volume chemical. (Commodity is represented by most basics and intermediates.) The commodity-type typically has a longer product life cycle than the specialty-type chemical.

k) The new chemical can be targeted cost-effectively to the entire U.S. market (vs. only regional, where plant is located.) (i.e., this analysis ignores the transportation cost effect when estimating market share, in order to assume the highest market share potential possible.)

l) Cost of selling varies from one category to the next, (packaging, distribution, form of product, variance in specifications, etc.) but is not considered as part of this procedure.

m) Concentration of users/purchasers/customers has an effect on market share potential. (If only one or two firms purchase the product vs. 100 or 200 it may be more difficult to penetrate the market. Some estimate of potential use will be provided in the PMN, however the reviewer must exercise judgement.)

n) Some firms identified as competitors may in fact have the capability to manufacture the chemical but may not currently be doing so. This can only be accurately determined by surveying the firms who are identified as competitors in the trade literature. Implicit in the fact as to whether a firm is large or small is whether the sales force is adequate, the production capacity is adequate, etc. with respect to the competition.

o) The firm planning to manufacture the new chemical is assumed to have a patent position at least for the first five years, thus implying that there are no others who could offer the identical product for several years. The actual length of time protecting a patent position in the market is based on the time used to obtain regulatory approval.

p) In general, factors which should be taken into consideration in any detailed analysis of a new product market potential can be represented by the following summary:

Initial Considerations--

- New Markets versus Existing Market
- Standarized versus Non-Standarized (i.e. Commodities vs. Specialties)
- Industrial versus Consumer (i.e. Basic, Intermediate, End)

Production--

- Raw Material Available/Cost
- Process Technology
- Experience
- Production Costs
- Scale of Production
- Forward/Backward Integration
- Capacity Utilization

Product--

- Quality and Specifications
- Pricing Policy (i.e. profit margins, competitive philosophy, etc.)
- Service

Market--

- Market Segment Sizes (Volumes) by Function
- Market Segment Sizes (Volumes) by Applications
- Market Segment Maturity (i.e. Stage in the Life Cycle)
- Market Segment Historical Growth
- Market Segment Competition
- Opportunity to Substitute for Non-Chemical-Derived Products (i.e. New Market or Existing Market Expansion)
- Price Elasticity of Demand (i.e. Commodity vs. Specialty)
- Rate of Product Acceptance within a Function/Application

External Variables--

- Impact of Imports/Exports
- The Economy
- Government Regulations
- Materials Availability
- Energy

EXAMPLE MARKET SHARE ESTIMATION

Chemical: Tris (2,3-dibromopropyl) phosphate

Function: Flame Retardant (Function Code No. 220)

Market Share Estimation:

- Fifth Year Market Share Estimate

Using $MS_{5nc} = abc\ MS_{bv}$,

where $MS_{bv} = .030$ ($25 < N_T \leq 50$ from Appendix A),

$a = 5$ (Assumes that the firm introducing the new chemical is large)

$b = 1$ (Assumes that the firm is currently in the flame retardant business),

$c = 1$ (Assumes chemical category is receptive to fairly rapid new product acceptance),

then $MS_{5nc} = 5x1x1x.030$

$$\underline{\underline{MS_{5nc} = .15 \text{ (or 15\%)}}}$$

- First and Third Year Market Share Estimate

Using $MS_{1nc} = d\ MS_{5nc}$,

where $MS_{5nc} = .15$,

$d = .2$ (From 5 year new product growth cycle)

then $MS_{1nc} = .2x.15$

$$\underline{\underline{MS_{1nc} = .03 \text{ (3\%)}}}$$

Similarly, $MS_{3nc} = e\ MS_{5nc}$

where $e = .8$ (From 5 year new product growth cycle)

then $MS_{3nc} = .8x.15$

$$\underline{\underline{MS_{3nc} = .12 \text{ (12\%)}}}$$

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SECTION 6

THE CORRELATION OF CHEMICAL STRUCTURE WITH PHYSICAL, CHEMICAL AND BIOLOGICAL PROPERTIES: APPLICATIONS IN EXPOSURE ASSESSMENT

Where there are gaps in the informational data base predictions based on judicious application of available correlations of chemical structure with physical, chemical and biological properties can contribute to the development of reasonable estimates of exposure levels. Such correlations can be helpful in developing predictions in the following areas relevant to exposure assessment:

a) Potential uses of a new chemical;

b) Potential for direct transport through the environment;

c) Potential for direct systemic uptake of the chemical by exposed humans;

d) Potential for formation of by-products, co-products and degradation products during manufacture and processing of the chemical and identification of such products;

e) Susceptibility to chemical and biological degradation in the environment and identification of degradation products; and

f) Potential for bioaccumulation.

The operative modifier, "judicious application," needs to be emphasized. In general, to derive meaningful predictions from structure-property correlation, the advice of consultants expert in the particular field should be sought.

POTENTIAL USES

The techniques of pattern recognition appear particularly well suited to the purpose of anticipating potential uses of a new substance.[1,2,3] Supplementary insight can be gained by a consideration of available information on physical and chemical properties. For computer operation, pattern recognition methods would require quite sophisticated hardware and software. At this time, the NIH-EPA Structure and Nomenclature Search System, which contains over 100,000 different compounds, might serve the purpose[10]. To fulfill the objective of defining potential uses, however, computer operation may not be necessary. Since an experienced chemist should be able to do the job and do it more quickly and economically.

The procedure would be essentially as follows:

a) Inspection of the molecular structure and the properties of the chemical;

b) Selection of information for similar structural patterns;

c) Identification of existing uses of compounds of like structure and properties;

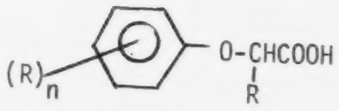
d) Estimation of the probable cost of manufacture of the new chemical and matching of manufacturing cost against the list of possible uses to assess market potential, and

e) Listing of potential uses of the new compound.

The Chemical Use List elaborated by the EPA[21] forms an excellent basis for the purpose of classifying potential uses of a new compound. In general, pattern recognition techniques would be better used in predicting "function" than "application" as defined in the EPA list.

It should be noted that estimation of the probable cost of manufacture can again be most conveniently done by an experienced chemist. Computer techniques, essentially based on pattern recognition but far more sophisticated still,[4-7] could conceivably be used for the mapping and costing of synthetic processes but at this time would certainly be unwidely, impractical and unnecessary.

The concept of pattern recognition is based on the observed relatively high probability that compounds with like structural patterns will have like properties. Chemists seeking to design new compounds having certain properties tend to use as a model an existing compound already known to have those properties. For example, with respect to identification of possible uses, if one discerns a substituted phenoxyacetic acid moiety in the molecular structure and there are few extraneous polar, functional or bulky groups present, one could conclude that the compound might find use as a herbicide.



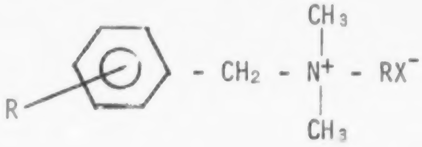
(possible herbicide) (1)

The conclusion would be reinforced if R = Cl. Depending on the nature of substituents, the compound might also have anti-inflammatory properties. Use as an anti-inflammatory agent would, however, be unlikely unless the company proposing to introduce the compound was in fact an ethical pharmaceutical house.

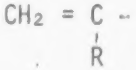
If a compound contained a long aliphatic hydrocarbon chain terminating in a highly polar group, either anionic, cationic or nonionic, depending on its lipophilic-hydrophilic balance, there would be a high probability the compound could find use as a detergent, surfactant, foam stabilizer, wetting agent, emulsifier, etc.

$R - (CH_2)_2 - X$ (possible surfactants, etc.) (2)
$X = -OCO - Na^+$ (anionic) (2a)
$X = -N(CH_2CH_2OH)_2$ (cationic) (2b)
$X = -C(=O) - N(CH_2CH_2OH)_2$ (nonionic) (2c)

An aralkyl quaternary ammonium salt[3] could be a bactericide, algicide, disinfectant, emulsion stabilizer, etc.


(possible bactericide, etc.) (3)

A relatively low molecular weight compound with an activated, terminal double bond[4] could serve as a polymerization intermediate.


$CH_2 = \underset{R}{C} - X$ (possible polymerization intermediate) (4)

A multitude of other examples could be cited but these should serve to illustrate the principle. It should be noted that pattern recognition can also be used to identify known analogs for which regulatory actions have already been taken.

Potential for Direct Transport

The extent to which a compound could be transported through the environment, and its distribution in the environment will depend on environmental conditions as well as upon on the following properties of the compound[8]:

a) Physical state (liquid, solid-(particle size), gas;

b) Volatility;

c) Density;

d) Lipophilic-hydrophilic balance;

e) Solubility in water;

f) Chemical stability.

Certain of these terms describe overlapping, but not precisely coincidental, features of a compound. For example, with respect to a), b), and c), a solid can have higher volatility and lower density than a liquid. With respect to d) and e), solubility of a solid in water will depend not only on lipophilic-hydrophilic balance but also on crystal lattice energy.

It is possible to make reasonable predictions of transport through the environment by means of mathematical-computer techniques. The limited amount of data on the properties of a new compound requires careful development of estimates.[8]

First, in order to be transported any distance from the source, the chemical must have sufficient chemical stability to survive the time it takes to migrate that distance. For purposes of this program, it was assumed that the compound would be sufficiently stable to be transported. A compound with a half-life of less than 12 hours might be considered to undergo breakdown sufficient to render stability a significant influence on direct transport.

Transport can occur through water and/or air; the material will be distributed in the air, water, and in and on solid surfaces (land). In addition to the physical and chemical nature of the compound, major determinants of the rate of transport and concentration at a given distance are factors external to the inherent properties of the substance, viz., rates of flow of air and water, volume of water, and ambient temperature. The properties of the molecule have the major influence on steady state concentrations of the substance in air, water and land therefore this discussion has been confined to consideration of steady state concentrations.

The steady state concentration in air of a solid at a distance from the source will be a direct function of its volatility, and inverse functions of its density, particle size and water solubility. The steady state concentration of a solid in water will be inverse functions of its volatility and its lipophilic-hydrophilic balance--which may be expressed in terms of partition coefficient between octanol and water[9]--and a direct function of its water solutibility. Concentration on land will be inverse functions of its volatility and water solubility and direct functions of its density and partition coefficient. Corresponding relationships can be formulated for liquids and gases.

Information as to the physical state of the materials, although possibly not the particle size of the solid, will certainly be available from the manufacturer. Data relating to volatility, density and water solubility may also be available, but, information with respect to lipophilic-hydrophilic balance may not be available.

Volatility is a property determined not only by the vapor pressure of the compound but also by its latent heat of vaporization and its partition coefficients between air and water and between air and soil. That is, the degree to which the compound is held, or possibly even complexed, in water or by soil will be important influences on the proportion of the substance released to air from the latter geospheres. Although information on vapor pressure may be available, data on the heat of vaporization and on air-water and air-soil partition coefficients will almost certainly not be available. Estimates can be made based on molecular weight, which will have an inverse relationship with volatility, presence of polar, hydrogen bonding and/or ionizable groups, which can have a profound effect in decreasing volatility.

Density of a gas can be simply estimated because gas density will vary directly with molecular weight. If we assume that there is no intermolecular association, (which is a reasonable approximation for a gas at low concentration), and that the substance obeys the ideal gas law, we can actually calculate the density based on the fact that 1 mole of a perfect gas occupies a volume of 22.4 liters at 0°C and 1 atmosphere pressure. Thus the density in grams/liter at standard temperature and pressure can be calculated:

$$d = \frac{\text{Mol. Wt.}}{22.414}$$

Density of a liquid may be estimated based on the fact that density will vary directly with degree of intermolecular association. Compounds without polar, hydrogen bonding, ionizable groups or available bonding electrons and bonding orbitals (e.g., saturated hydrocarbons) will have a low density (<1). Density will increase with the introduction of groups capable of entering into progressively stronger intermolecular bonding interactions. Fluorocarbons, presumably because the fluorine atom holds its electrons very tightly and is unwilling to share them, are nearly equivalent to hydrocarbons in their low density and high volatility. Other halocarbons, chloro, bromo and iodo derivatives, do enter into intermolecular associations and have very high densities and low volatility. As a general rule, the heavier elements, elements of the second row of the periodic table and beyond, with unsatisfied outer shells, are more capable of entering into intermolecular bonding associations than are the lighter elements.

Density of a solid is much more difficult to predict because it depends so much on the crystal structure--the distance between molecules in the crystal lattice. Moreover, a solid can have more than one crystal structure. The morphology of its crystals, and therefore their density, can vary depending on the conditions of formation. Estimates can best be made on the densities of the most closely analogous compounds.

There is considerable information concerning the lipophilic-hydrophilic balance of organic molecules which is expressed in terms of the partition coefficient (P) between 1-octaonol and water. The partition coefficients of a large number of compounds have been determined and tabulated.[9,11-14] Also tabulated are a large number of substituent constants (Π) which indicate the effect of a particular substituent on the partition coefficient of a parent molecule.[9,11-13,15-17,32] To calculate an approximate partition coefficient for a new compound, the value(s) of the relevant substituent(s) are added to the log P of the most closely related parent compound for which data are available, and the antilog of the sum is determined:

$$Px = \text{Antilog}\ (\Pi_{s-_1} + \Pi_{s-_2} + \Pi_{s-n} + \log Po)$$

Px is the partition coefficient of the new compound, Po is the coefficient of the closest known parent compound and Π_{s-n} is the substituent constant of the nth substituent. The more closely related the substituent(s) and the parent compound are to the new compound the more confidence one can have in the validity of the calculated partition coefficient. The larger the partition coefficient, the more lipophilic the substance and the less its compatibility with aqueous systems. Polar, hydrogen bonding and ionizable groups will lower partition coefficients.

The partition coefficient may be used to estimate the water solubility of a liquid or a gas. The smaller the partition coefficient, the greater the water solubility. The solubility of compounds with acidic or basic groups will be markedly affected by the pH of the aqueous medium. That is, a substance with a low pKa (acid) will be solubilized in water at a high pH (alkaline) whereas the converse will be true of a substance with a high pKa (base). The solubility of gases and liquids with a high vapor pressure at ambient temperature decreases with increasing temperature whereas the solubility of liquids with low vapor pressure (and solids) usually, but not always, increases.

The water solubility of a solid also depends on its partition coefficient and on the presence or absence of acidic or basic functions. In addition the water solubility of a solid can be markedly influenced by its crystal lattice energy. For example, the stronger the forces stabilizing the crystalline form, the more the thermodynamic equilibrium between the crystalline solid and dissolved solid will be shifted toward the crystal. Dipolar ionic substances, for example amino acids, have much lower solubilities in water than would be expected on the basis of their polarity, presumably because of electrostatic stabilization of the crystal lattice. Solubility can be markedly increased in a medium that is sufficiently acid or alkaline to convert the charge-neutralized molecule to a salt form.

Chemical stability in the context of environmental degradation will be discussed in a later section.

To estimate the effect of the chemical properties on the direct transport and distribution of a substance, one should collect available data on the physical state, volatility, density, lipophilic-hydrophilic balance, water solubility and, if the compound is likely to be very unstable, its chemical stability. Estimates of direct transport can then be made based on data available for known compounds.

POTENTIAL FOR DIRECT SYSTEMIC UPTAKE

Exposed humans may take in a chemical by absorption through the skin or other membranes, by inhalation and/or by ingestion through the gastrointestinal tract. The proportionate amount of a dose of a chemical an exposed human recieves will depend on the route(s) of uptake and on the properties of the substance.

The skin and other external membranes are basically composed of layers of lipids with thin water-soluble polar groups facing outward and their non-polar carbon chains held together on the inside.[18-20] The lipid layers are stabilized by layers of protein molecules. It is believed that large numbers of tiny water-filled chemicals or pores are distributed throughout these membranes. The presence of pores is inferred from the behavior of the membranes; the effective pore size appears to be about 4Å. The main difference between the skin and other outer membranes (of the mouth, nasal cavities, etc.) is that the skin has an additional outer, horny layer densely packed with keratin (a protein). Rates of absorption through the skin are slower than through other external memberanes and varies qualitatively with variations in properties of the substances being absorbed.

Most foreign substances are absorbed through these membranes by passive diffusion processes.[18-20] The ability of substances to diffuse through the skin is directly proportional to their lipophilic-hydrophilic balance, i.e., their octanol-water partition coefficient. The more lipophilic the substance, the better it will be absorbed. It should be noted that extremely lipid-soluble materials will rapidly diffuse into the membrane but then be held in the lipid layer and diffuse into the systemic circulation only slowly. Highly polar, lipid-insoluble substances cannot be absorbed through the skin unless their molecular size is small enough, no more than the equivalent of about a 3-carbon atom chain (or 4Å), to pass through the presumed water-filled channels.

Particle size will markedly influences absorption through the skin. In order to be absorbed by passive diffusion, a substance must not only be lipid-soluble but must be in a form available for dissolution in the lipid layer. Thus the rate of absorption will vary inversely with particle size.

A substance will usually enter the gastrointestinal tract via the oral route. From the mouth, where the pH is approximately neutral, a substance will pass into the acid milieu (pH 1-4) of the stomach, thence to the small intestine, where the pH again approaches neutrality, and finally to the large intestine. Systemic absorption can take place in any of these regions but the major fraction of the absorption generally takes place in the small intestine.

The principles governing absorption of foreign substances from the gastrointestinal tract are the same as for absorption through the skin and other membranes.[18-20] Absorption is generally by pasive diffusion and absorbability varies directly with octanol-water partition coefficient. Acids and bases will more readily pass through the wall of the gastrointestinal lumen in their unionized form. Therefore, bases, which will normally exist in the protonated ionic form in the acid environment of the stomach, will be largely absorbed from the intestines whereas lipid-soluble acids and neutral molecules can be abosrbed from the stomach. Highly polar substances will not be absorbed unless they are small enough to pass through the water-filled channels or, in exceptional cases, are carried across by active transport. Active transport processes will be available only to substances closely resembling normal substrates (e.g., glucose, L-amino acids, uracil).

Degree of absorption of a solid will vary inversely with particle size. In order to be absorbed, a lipid-soluble substance must be in a form available for dissolution in the lipid layer of the intestinal wall.

Since the stomach provides a strong acid environment and the entire gastrointestinal tract provides a variety of digestive enzymes capable of breaking down proteins, carbohydrates and neutral fats and the colon contains colonies of bacteria capable of effecting a range of chemical transformations, one must consider the possbility that an ingested substance, itself unable to be absorbed, might be susceptible to degradation to absorbable breakdown products. Acid-labile substances, protein-like or carbohydrate-like materials, and high molecular weight esters should be evaluated in this context.

It should be noted that a substance absorbed from the gastrointestinal tract will normally immediately enter the portal circulation and be channeled directly to the liver where it could undergo degradation by microsomal enzymes.

Substances present in the air, i.e., gases, volatile compounds and aerosols can be inhaled into the lungs. Ability of aerosols to reach the lungs depends on particle size (Table 8).[20] Large particles (>10 microns) are almost completely retained in the nasal passages. As the particles become smaller, increasing proportions will reach the alveoli. Insoluble particles retained in the upper respiratory tract are rapidly cleared by a mucous blanket which covers the tract down to the terminal bronchioles and which is propelled upward by ciliary movements.

TABLE 8. PERCENT RETENTION OF INHALED AEROSOL PARTICLES

Particle Size, μm	Percent Retention in Nasal Passages
>10	∿100
5	50
2	20
<1	0

Absorption of materials reaching the lower respiratory tract and the alveoli can be extremely rapid. The rate of absorption into the systemic circulation through the alveolar endothelium is influenced by the properties of the sbustance being absorbed in the same manner as through other biological membranes. Absorption rate increases with increasing octanol-water partition coefficient and with decreasing particle size.

The process for estimating the effect of chemical properties on systemic uptake of a new substance by exposed humans may be generically illustrated as in Figure 11.

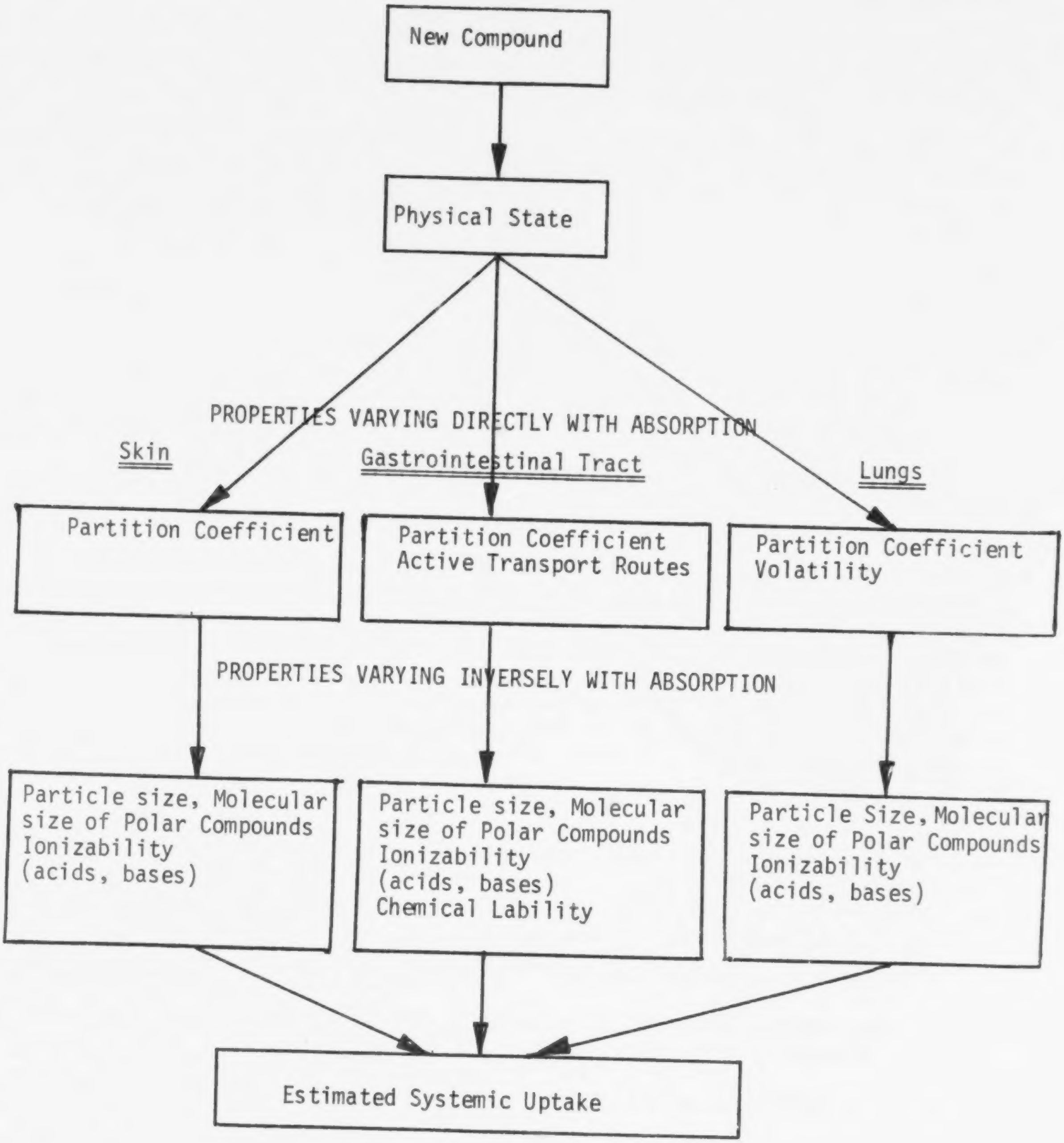

New Compound
Physical State
PROPERTIES VARYING DIRECTLY WITH ABSORPTION
Skin
Gastrointestinal Tract
Lungs
Partition Coefficient
Partition Coefficient
Active Transport Routes
Partition Coefficient
Volatility
PROPERTIES VARYING INVERSELY WITH ABSORPTION
Particle size, Molecular size of Polar Compounds
Ionizability
(acids, bases)
Particle size, Molecular size of Polar Compounds
Ionizability
(acids, bases)
Chemical Lability
Particle Size, Molecular size of Polar Compounds
Ionizability
(acids, bases)
Estimated Systemic Uptake

Figure 11. Effect of chemical properties on systemic uptake.

POTENTIAL FOR BY-PRODUCT FORMATION

Estimation of the potential for formation of by-products and degradation products during manufacture and processing, and prediction of the identity of such products will be required for adequate premanufacture review.

With respect to manufacture, one must first define the synthesis route being used, starting materials, reagents, conditions, and purification procedures. Some information as to the method of synthesis may be supplied by the chemical manufacturer but surely not precise details of conditions used and in-plant operational procedures. Information not supplied will have to be estimated. Since there is generally more than one potentially useful route to a compound and since other manufacturers might choose to go into production, one will have to identify and evaluate alternative syntheses. Thus, before beginning to estimate possibilities for by-products formation, one must:

a) review supplied information on the existing, syntheses route;

b) estimate or obtain operational details that are not supplied;

c) identify and evaluate alternative syntheses.

Given the syntheses route, it will be possible to make reasonable estimates of the conditions used and of operational procedures. Potential alternative syntheses may be identified by pattern recognition techniques as discussed earlier. In its simplest form, this would entail reviewing a suitable data base such as the NIH-EPA Structure and Nomenclature Search System for compounds with a similar molecular structure. Sophisticated computer techniques have been developed for the purpose of syntheses analysis[5-7] but do not appear to have evolved to the point where they would be useful for the present purpose.

This information can be used to predict the principal kinds of by-products, co-products and degradation products that could form during manufacture and be present in process streams and/or the final product. Predicting of the by-products which may be formed in trace amounts will be difficult if not impossible at this point.

With respect to processing, one must consider:

a) the chemical properties, especially the stability of the compound;

b) the conditions of processing for the existing use; and

c) potential additional processes in which the compound might be used.

By inspection of the structure of the compound, consideration of the functional groups and the existence of labile features, it is possible to predict the stability and the conditions under which it might degrade as well as the products that might be formed. Although there is always the possibility that unanticipated trace and/or unobvious degradation products can be formed, reasonably accurate predictions are possible. For example, if the compound has an unhindered ester function with some water solubility and is to be heated in water during processing, the possiblity of hydrolysis of the ester group is obvious. If the compound has an allylic alcohol grouping and is treated with acid during processing, there are the possibilities for dehydration and/or rearrangement depending on the molecular structure. There is also the possibility of air oxidation. If the compound is a silver salt, there are possibilities for deposition of silver oxide, or, in the presence of a reducing substance, free silver.

Some information regarding processing for proposed uses, e.g., as a pigment in the formulation of paints, as a foam stabilizer for foamed rubber, as a gelling agent for adhesives, etc., may be supplied but details of processing conditions probably will not be supplied. General knowledge of the type of processing and discussion with users can be used to make reasonable estimates for processing conditions.

For the purpose of predicting additional processes in which the compound might be used, it will be necessary to:

a) predict other applications where the compound may be used and

b) judge if the compound might have other potential functions and consequent applications.

The physical and chemical properties of the compound can be used to predict applications where the compound might have utility. With the aid of pattern recognition techniques, and suitable data base such as that already referenced, one can identify known compounds having analogous molecular arrangements and similar properties. Based on the functions and applications of these known materials and with the aid of the Chemical Use List published by the EPA, one can project potential additional uses of the new compound. Processing conditions can then be estimated for these additional application areas. With these estimates in hand, projections can be made of degradation products that might form during processing.

SUSCEPTIBILITY TO ENVIRONMENTAL DEGRADATION

In evaluating the susceptibility of a compound to chemico- and biodegradation in the environment, it is necessary to consider its structure, physical and chemical properties, and the physical, chemical and biological stresses to which it will be exposed. Physical and chemical forces in the environment that might cause degradation include: heat, ultraviolet radiation, oxygen, water, acid, alkali, oxidizing systems, and reducing systems. Biodegradation could result from uptake by microorganisms, insects, fish, birds, mammals, and could involve successive ingestion through the biological chain.[8]

From inspection of the molecular structure of a new compound, it is possible to predict the physical and chemical forces in the environment which may affect it and to predict probable products. From the physical characteristics, water solubility, partition coefficient, and volatility, a prediction of the distribution of the compound in the environment is possible. This effort can be supplemented by a computerized pattern recognition search of a data base in order to identify compounds possessing analogous structural features and functional groups for which environmental fate has been studied. Frequently sufficient literature data are available to enable the development of reasonably quantitative estimates of rates of degradation.

For example, considerable information is available on the effects of substitution on the susceptibility of benzene and its derivatives to physical and chemical actions in the environment.[22-25] Benzene itself is not susceptible to degradation by water, acid, alkali or reducing systems under environmental conditions and is substantially more stable than other hydrocarbons to oxidative and photochemical degradation. The effects of substitution on oxidative degradation are consistent with electrophilic attack on the beneze ring. Thus, introduction of electron-donating substituents--alkyl, hydroxy, amino--markedly enhances substituents such as chloro or bromo and further stabilize the ring to oxidative attack. Of course, the substituent itself can be sensitive or engender lability to other agents, e.g., the sensitivity of nitrotoluenes and of phenols to alkali. Chlorinated aromatics are subject to photochemical dechlorination; for example, the polychlorodibenzodioxins are dechlorinated by sunlight when present in very thin films or dilute solutions but are otherwise extremely resistant to attack.[24-25]

Estimates of possible biodegradation can be made by experts in the areas of microbiology and biochemistry. Knowledge of the molecular structure of the new compound, its physical and chemical properties, coupled with knowledge of the possibilities for uptake by micro- and macro-organisms and of the metabolic pathways available to these organisms[26], will permit estimation of susceptibility to metabolic degradation and the probable products of such degradation. A pattern recognition search to identify compounds with similar structural features and for which information on biodegradation is available can be used to assist in development of predictions. The rate of biodegradation can be expected to be much more sensitive to subtle changes in structure, steric factors, and lipophilic hydrophilic balance than would the rate chemical degradation.

In order to be metabolized a compound must first be taken up by the organism. This uptake requires penetration of biomembranes and follows the same general rules discussed for human uptake. In addition, microorganisms can take in foreign bodies by engulfing them (pinocytosis). A high octanol-water partition coefficient will generally favor uptake. Microorganisms can take up substances by means other than absorption through a biomembrane, and have great versatility in their ability to metabolize foreign compounds. The metabolized products may then be in a form more readily absorbed by higher organisms (for example, the conversion by some bacteria of mercury to the readily absorbable methylmercury and dimethylmercury). Thus it is not possible to rule out absorption of a compound simply because in its unmetabolized form it would be incapable of absorption through membranes.

Once absorbed, the metabolic processes to which a compound would be subjected will depend on its distribution in the organism and its ability to reach the appropriate enzyme systems. While distribution will not be a factor with microorganisms, it can have major significance with higher organisms. A compound with a lipophilic-hydrophilic balance in an intermediate range can concentrate in the liver, gain ready access to the microsomal enzymes contained therein, and then be a candidate for metabolic degradation. A highly polar substance may be rapidly excreted unchanged through the kidneys whereas an extremely lipophilic compound may be stored in the fat and released slowly, if at all, into the circulatory system where it can be brought into contact with metabolic enzyme systems.

In general, metabolic processes convert lipophilic substances into less lipophlic, more polar products.[26] These metabolic products are usually, but not always, less toxic than their parents.

Microorganisms are extremely versatile in their metabolic abilities: they have a broad array of metabolic enzyme processes at their disposal and frequently can develop enzyme systems to metabolize compounds that they were originally unable to handle.[28] Nevertheless, microorganisms have their limitations. For example, bacteria that produced adaptive enzymes to degrade a specific phenolic compound were readily able to metabolize a variety of phenols, benzoic acids and benzaldehydes but had little or no ability to metabolize benzene, toluene, nitrobenzene or halogenated aromatic compounds.[28]

Metabolic processes that can be effected by mammalian systems include:[26,29]

1) Oxidation by microsomal enzymes
    a) epoxidation and hydroxylation of aromatic compounds
    b) hydroxylation of alkyl chains
    c) deamination
    d) N-dealkylation
    e) O-dealkylation
    f) N-oxidation
    g) S-oxidation

2) Reduction by microsomal enzymes
    a) reduction of azo and hydrazo groups
    b) reduction of nitro groups

3) Other oxidative systems
    a) aromatization
    b) oxidation of alcohols and reduction of aldehydes and ketones
    c) oxidation of aldehydes

4) Hydrolysis of esters and amides

5) Conjugation
    a) formation of glucuronides
    b) formation of sulfate esters

c) mercapturic acid conjugation
d) methylation
e) acylation

6) Covalent binding to tissue proteins and/or nucleic acids

Clearly, an absorbed compound will be subjected to a broad range of metabolic processes. Most of these will produce more polar substances which can be excreted. Obvious exceptions are processes resulting in covalent bond formation with proteins and nucleic acids. Such bond formation can occur if the compound has an electrophilic center, or has an electrophilic center metabolically generated, which is sterically accessible for binding to a nucleophilic site on biopolymers. Chloromethyl methyl ether is an example of a direct alkylating agent. Dimethylnitrosamine and benzo(a)pyrene are examples of compounds which are first oxidized by microsomal enzymes to generate species capable of covalent binding to nucleophilic sites.[27,28]

Compounds with an appropriate lipophilic-hydrophilic balance, having the kinds of structural features or functions which would be susceptible to attack in any of the listed enzymatic processes and which are not sterically inaccessible, can be expected to be metabolized after absorption. To be susceptible to attack by an oxidative enzyme, the compound whould be readily capable of donating electrons to the enzymatic acceptor. Thus aromatic compounds with electron-donating substituents (e.g., acetanilide) are readily enzymatically oxidized whereas those with electron-withdrawing groups (e.g., halogenated aromatics) are resistant to metabolic oxidation. For enzymatic reduction on the other hand, the compound must have groups able to accept electrons (e.g., the nitro group of nitrobenzene). For conjugation, a compound must have a group capable of being conjugated (e.g., hydroxyl, amino, sulfhydryl). A compound can undergo sequential attack by a series of enzyme systems, for example: hydrolysis of an ester followed by oxidation of the resultant aniline; hydroxylation of an alkyl group followed by conjugation of the alcohol.

POTENTIAL FOR BIOACCUMULATION

In order for a compound to have a potential for bioaccumulation, be resistant to chemico- and bio-degradation and thus be persistent in both geo- and bio-spheres; it must be capable of undergoing uptake by living organisms, and must be resistant to excretion.[8]

Compounds resistant to chemico- and bio-degradation in the environment will be those having attributes to discussed previously such as resistance to the physical, chemical and biochemical processes with which it may come in contact. Thus stable compounds that do not have structural features subject to ready breakdown are candidates for bioaccumulation.

To be capable of undergoing uptake by living organisms, compounds must either: a) have some degree of lipid solubility; b) if highly polar, be extremely small in molecular size; or c) be subject to active transport. Highly polar compounds will be excreted, unchanged and/or metabolized, about as rapidly as they are taken in and thus generally will not be subject to bioaccumulation. A compound taken in by an active transport process, since it will resemble a normal substrate, would be expected to follow the metabolic and excretary pathways of the prototype and thus not, itself, be accumulated although a metabolite could emulate the normal metabolite and be incorporated into biopolymers.

Resistance to excretion normally requires an extremely lipophlic molecule which will be distributed to, and stored in, fatty tissues where it will not suffer enzymatic breakdown and from which it will be released only slowly.

In general, compounds that will be subject to bioaccumulation are chemically and biochemically stable, highly lipophilic substances. Typical of such compounds are certain halogenated aromatic hydrocarbons, well-known illustrations of which are DDT and PCB's.[30] The potential for the bioaccumulation of halogenated aromatic hydrocarbon depends on their degree of lipophilicity, which determines their relative distribution between the fat and the liver, and the number and exact positions of their halogen substituents, which largely determines their chemical stability and lack of susceptibility to microsomal enzymes. Birds and fish appear to be particularly subject to bioaccumulation of stable, lipophilic compounds like the halogenated aromatic hydrocarbons.

In addition to stable, lipophilic molecules which may be distributed to adipose tissue and there accumulate without undergoing chemical transformation, certain compounds may, in the course of undergoing transformation, become covalently bound to biopolymers, and thus not the compounds themselves but their metabolic products may be bioaccumulated. As mentioned earlier, compounds closely resembling normal substrates may suffer such a fate by being incorporated into biopolymers in place of the normal substrate. A more common possibility, is that of a compound, such as any carcinogen whose mechanism of action has been elucidated, being itself capable of forming covalent bonds with nucleophilic sites on biopolymers or of being converted into a metabolite capable of such action. It should be noted that this route of accumulation, through covalent bonding to a biopolymer, would only be accumulation in the individual organism and would not result in bioaccumulation through the food chain. This is so because the higher organism ingesting the substituted biopolymer would have to break it down before absorbing it and the resulting fragments would no longer be likely covalent bond-forming agents. Thus one may distinguish between individual bioaccumulation and bioaccumulation in the food chain.

A procedure for conducting the bioaccumulation prediction is represented schematically in Figure 12.

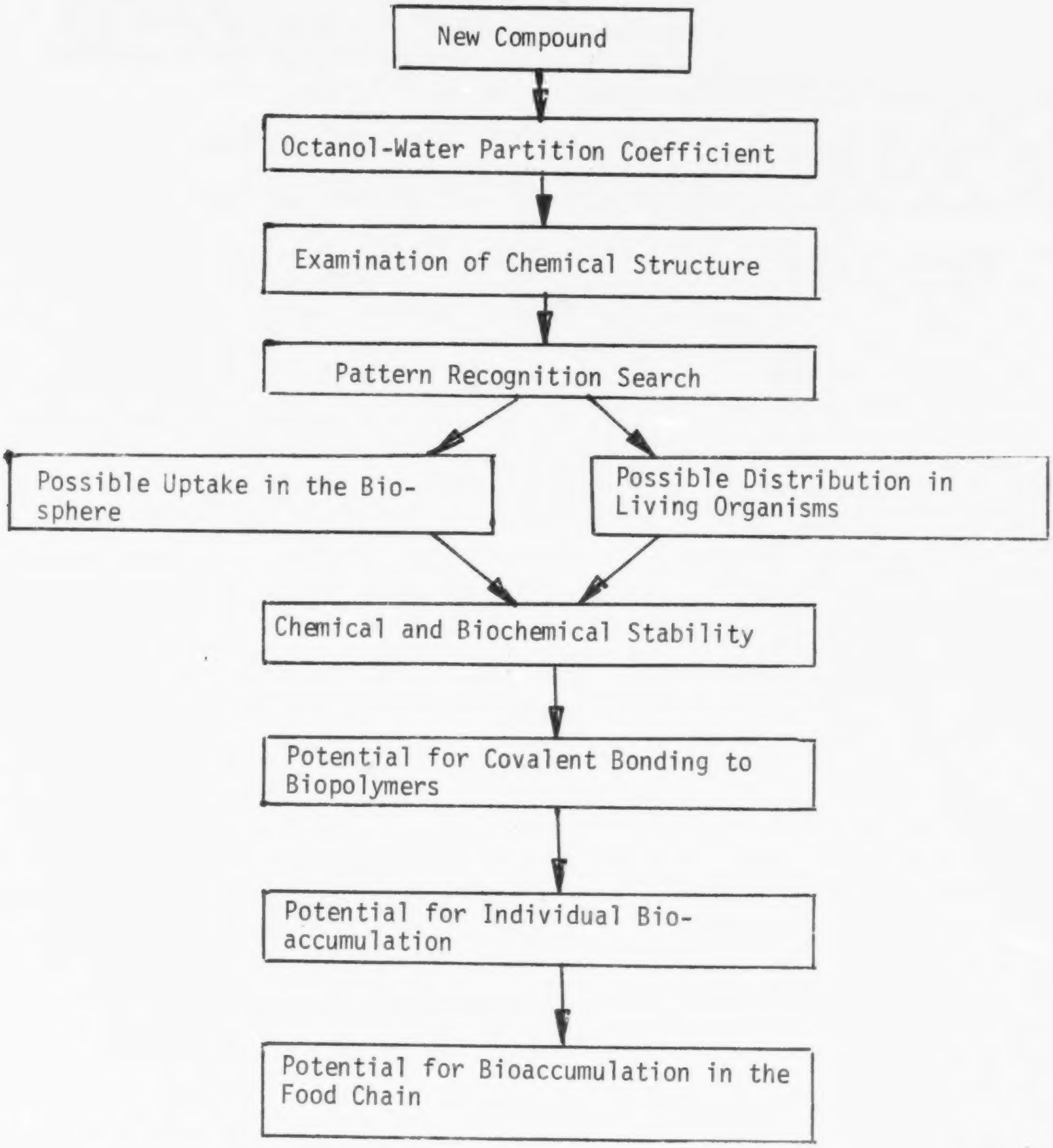

New Compound
Octanol-Water Partition Coefficient
Examination of Chemical Structure
Pattern Recognition Search
Possible Uptake in the Biosphere
Possible Distribution in Living Organisms
Chemical and Biochemical Stability
Potential for Covalent Bonding to Biopolymers
Potential for Individual Bioaccumulation
Potential for Bioaccumulation in the Food Chain

Figure 12. Potential for bioaccumulation.

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INFORMATION SOURCES

The most generally useful sources of information on the chemical properties of compounds were:

1. The Merck Index.

2. Handbook of Chemistry and Physics (particularly for data on vapor pressure at different temperatures).

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5. Manufacturers' technical bulletins.

6. Personal knowledge.

SECTION 7

APPLICATION OF PROCEDURE

The procedures discussed in the previous sections were applied to 30 chemicals selected by the EPA. This list included some well established chemicals in addition to chemicals produced in the small volumes expected for the pre-manufacturing notice chemicals. Since the procedures were developed for small volume chemicals there was some difficulty when they were applied to large volume chemicals that have many different uses; in these cases (benzene, acetone, etc.) the results are illustrative only, and not definitive. In all cases expert judgement was required.

The estimated physical and chemical properties of the chemicals were obtained and are given for each chemical in the appendix.

These data, along with potential use data and market data were used to estimate production volumes, number of plants and number of processing steps. The estimated market share for each of the 30 chemicals for the 1st, 3rd, and 5th year are given in Table 9.

Table 10 lists the predicted number of manufacturing personnel and the predicted concentration of the chemical in the work space. This table also lists the number of people and the concentration of the chemical in the vicinity of the plant.

Table 11 lists the consumer dose for the 30 chemicals. Of these chemicals, 8 were predicted to lead to no direct consumer exposure because they would be completely reacted during industrial processing (chemical intermediates) or because they would be contained within closed industrial cycles (catalysts).

For inhalation, most of the remaining chemicals were predicted to lead to dose by volatilization (about 8 have negligible diffusivity) and virtually all to dose via aerosols. Naturally, the inhalation route is very significant in direct exposure for high vapor pressure solvents that are rapidly volatilized, but it can be equally significant for low vapor pressure chemicals that are kept in the home a long time. The significant parameter is the ratio between the time over which the chemical takes to volatilize (Trel) and the product lifetime in the home (Ta + Tp). The yearly inhalation doses are conservative by a factor of about 10 because no allowance has been made for inhaled chemical that is later exhaled. Some evidence shows that the capture or retention efficiency of the lungs commonly ranges between 10 and 100 percent (Astrand 1978). Thus, for example, though the model predicts a probable average inhalation dose of 865 g of acetone to home house painters, the actual average might be aslow as 86 g due to this factor. Also, the inhalation dose is uncertain by virtue of the chemical diffusivity, and separate calculations have been done for minimum and maximum estimated values.

For contact, about 7 chemicals lead to no dose because one or more of the following parameters are effectively zero: water solubility, diffusivity, duration of skin contact and liquid-water penetration (a function of partition coefficient). Contact dose is usually most significant for chemicals with only low inhalation exposure, as otherwise the inhalation route would deliver a larger dose. Wherever data were not available, worst case assumptions are made (i.e. partition coefficient, solubility, etc.).

TABLE 9. MARKET SHARE FOR SAMPLE "NEW" CHEMICALS

Sample Chemical No.	Name	Function Code	No. of Competitors: Range	MS_{bv}	a	b	c	$MS_{s_{rc}}$	d	$MS_{1_{rc}}$	e	$MS_{3_{rc}}$
1	Tris (2,3 dibromopropyl Phosphate) Carpet Manufacture	220	25 - 50	0.030	5	1	1	0.15	0.2	0.03	0.8	0.12
2	Benzene	1211	51 - 100	0.0125	5	1	0.5	0.03	0.05	2×10^{-3}	0.25	0.01
		318	25 - 50	0.030	5	1	0.5	0.08	0.05	4×10^{-3}	0.25	0.02
		352	100⁺	0.005	5	1	0.5	0.01	0.05	5×10^{-4}	0.25	3×10^{-3}
3	Asbestos Cement Pipe Manufacture	2602	1 - 25	0.065	5	1	0.5	0.16	0.05	0.01	0.25	0.04
4	Ethylene dichloride	1211	51 - 100	0.0125	5	1	0.5	0.03	0.05	2×10^{-3}	0.25	0.01
		352	100⁺	0.005	5	1	0.5	0.01	0.05	5×10^{-4}	0.25	3×10^{-3}
5	Acrylonitrile	1211	51 - 100	0.0125	5	1	0.5	0.03	0.05	2×10^{-3}	0.25	0.01
		1212	26 - 50	0.030	5	1	0.5	0.08	0.05	4×10^{-3}	0.25	0.02
		299	1 - 25	0.065	5	1	0.5	0.16	0.05	0.01	0.25	0.04
6	Benzidine Yellow	1330	26 - 50	0.030	5	1	0.5	0.08	0.05	4×10^{-3}	0.25	0.02
7	Uni-Rez 2642	009	100⁺	0.005	5	1	0.5	0.01	0.05	5×10^{-4}	0.25	3×10^{-3}
8	Oil of Cedar leaf Flavor Uses	-	100⁺	0.005	5	1	1	0.03	0.2	0.01	0.8	0.02
9	2-benzothiazole-sulfonamide, N-(1,1-dimethylethyl)	1211	51 - 100	0.0125	5	1	0.5	0.03	0.05	2×10^{-3}	0.25	0.01
10	3-nitro Isatoic anhydride	1211	51 - 100	0.0125	5	1	0.5	0.03	0.05	2×10^{-3}	0.25	0.01
11	Dimercaptothiadiazole Formulated to Cutting Oils	1211	51 - 100	0.0125	5	1	0.5	0.03	0.05	2×10^{-3}	0.25	0.01
		1212	26 - 50	0.030	5	1	0.5	0.08	0.05	4×10^{-3}	0.25	0.02
		381	1 - 25	0.065	5	1	1	0.16	0.2	0.03	0.8	0.14
12	Adipic acid -1,4-butanedoil - 4,4'-diphenyl methane diisocyanate	009	100⁺	0.005	5	1	0.5	0.01	0.05	5×10^{-4}	0.25	3×10^{-3}
		132	100⁺	0.005	5	1	0.5	0.01	0.05	5×10^{-4}	0.25	3×10^{-3}
		211	1 - 25	0.065	5	1	1	0.33	0.2	0.07	0.8	0.26
		304	26 - 50	0.030	5	1	1	0.15	0.2	0.03	0.8	0.12
13	Benzyl trimethyl ammonium methoxide	112	50 - 100	0.0125	5	1	0.5	0.03	0.05	2×10^{-3}	0.25	0.01
14	Nitride DMTD	319	1 - 25	0.065	5	1	0.5	0.16	0.05	0.01	0.25	0.04
15	Strontium titanate	-	-	-	-	-	-	-	-	-	-	-
16	Acetone	1211	51 - 100	0.0125	5	1	0.5	0.03	0.05	2×10^{-3}	0.25	0.01
		318	26 - 50	0.030	5	1	0.5	0.08	0.05	4×10^{-3}	0.25	0.02
		352	100⁺	0.005	5	1	0.5	0.01	0.05	5×10^{-4}	0.25	3×10^{-3}
		3581	25 - 50	0.030	5	1	0.5	0.08	0.05	4×10^{-3}	0.25	0.02
17	Styrene Polysulfide	-	-	-	-	-	-	-	-	-	-	-
18	Hydrogenated Tallow Acids, ethanol amine condensate, ethoxylated	-	-	-	-	-	-	-	-	-	-	-
19	Surfynol 104(2,4,7,9-tetramethyl)-4,7 dihydroxy-deca-5-yne)	150	50 - 100	0.0125	5	1	1	0.06	0.2	0.01	0.8	0.05
		3620	50 - 100	0.0125	5	1	0.5	0.03	0.05	2×10^{-3}	0.25	0.01
		3621	50 - 100	0.0125	5	1	0.5	0.03	0.05	2×10^{-3}	0.25	0.01
		3627	50 - 100	0.0125	5	1	1	0.06	0.2	0.01	0.8	0.05
20	Allyl alcohol-Styrene Copolymer	128	26 - 50	0.030	5	1	0.5	0.08	0.05	4×10^{-3}	0.25	0.02
		132	100⁺	0.005	5	1	0.5	0.01	0.05	5×10^{-4}	0.25	3×10^{-3}
		213	50 - 100	0.0125	5	1	1	0.06	0.2	0.01	0.8	0.05
		304	26 - 50	0.030	5	1	1	0.15	0.2	0.03	0.8	0.12
21	Benzenediazonium, 2,5-dibutoxy-4-(4 morpholinyl)-sulfate	1330	26 - 50	0.030	5	1	0.5	0.08	0.05	4×10^{-3}	0.25	0.02
22	n-butylethyl-magnesium	112	50 - 100	0.0125	5	1	0.5	0.03	0.05	2×10^{-3}	0.25	0.01
23	Amberlyst Resin Catalyst	112	50 - 100	0.0125	5	1	0.5	0.03	0.05	[illegible]	0.25	0.01
24	Raney Nickel	112	50 - 100	0.0125	5	1	0.5	0.03	0.05	2×10^{-3}	0.25	0.01
25	Phosphorodithioic acid, S,S'-(thiodi-4,1-phenylene)	299	1 - 25	0.065	5	1	0.5	0.16	0.05	0.01	0.25	0.04
26	Hexachlorobenzene	1211	51 - 100	0.0125	5	1	0.5	0.03	0.05	2×10^{-3}	0.25	0.01
		236	26 - 50	0.030	5	1	0.5	0.08	0.05	4×10^{-3}	0.25	0.02
27	Trichloroethylene	1211	51 - 100	0.0125	5	1	0.5	0.03	0.05	2×10^{-3}	0.25	0.01
		153	1 - 25	0.065	5	1	0.5	0.16	0.05	0.01	0.25	0.04
		318	26 - 50	0.030	5	1	0.5	0.08	0.05	4×10^{-3}	0.25	0.02
		352	100⁺	0.005	5	1	0.5	0.01	0.05	5×10^{-4}	0.25	3×10^{-3}
28	Sulfuric acid	302	1 - 25	0.065	5	1	0.5	0.16	0.05	0.01	0.25	0.04
		318	26 - 50	0.030	5	1	0.5	0.08	0.05	4×10^{-3}	0.25	0.02
29	Iron (II) Sulfide	1331	50 - 100	0.0125	5	1	0.5	0.03	0.05	2×10^{-3}	0.25	0.01
		195	1 - 25	0.065	5	1	0.5	0.16	0.05	0.01	0.25	0.04
		272	100⁺	0.005	5	1	0.5	0.01	0.05	5×10^{-4}	0.25	3×10^{-3}
		318	26 - 50	0.030	5	1	0.5	[illegible]	0.05	4×10^{-3}	0.25	[illegible]

TABLE 10. MANUFACTURING EXPOSURE FOR SAMPLE "NEW" CHEMICALS

No.	Name	Production kg/yr	No. of plants	Max daily prod. kg (plant)	Persistence	Operator Exposure		Plant Vicinity Exposure 1.0 km Radius		2.0 km Radius		5.0 km Radius	
						Number	mg/m^3	Number	mg/m^3	Number	mg/m^3	Number	mg/m^3
1	Tris (2,3 dibromopropyl Phosphate)	4.07×10^6	1	11,300	1	11	0.8	3,660	0.117	14,600	0.035	91,400	0.007
	Carpet Manufacture	2.95×10^7	10	8,000	3	169	1.0						
2	Benzene	4.67×10^9	34	380,000	1	1350	0.89	124,000	3.9	496,000	1.2	3,108,000	0.20
	Benzene to Styrene	2.10×10^8	15	38,900	1	574	0.86						
3	Asbestos	8.76×10^7	7	49,700	3	176	2.6						
	Cement Pipe Manufacture	2.10×10^8	14	60,000	3	371	2.23	51,000	0.6	204,000	0.18	461,000	0.088
4	Ethylene dichloride	3.90×10^9	18	600,000	1	314	0.87	66,000	6.2	263,000	1.9	1,645,000	0.4
	Et. Dichloro to Vinylchloride	7.70×10^7	48	214,000	1	1335	0.89						
5	Acrylonitrile	6.90×10^8	6	320,000	1	274	0.89	22,000	3.33	88,000	0.99	548,000	0.20
6	Benzidine Yellow	6.80×10^5	4	640	3	31	0.92	14,600	0.07	58,400	0.02	366,000	0.004
7	Uni-Rez 2642	1.00×10^4	1	100	3	5	0.20	3,660	0.001	14,600	0.0003	-	-
8	Oil of Cedar leaf	4.50×10^3	2	75	1	10	0.05	7,300	0.0008	29,200	0.0002	-	-
	Flavor Uses	9.00×10^5	100	360	1	172	0.001	-					
9	2-benzothiazole-sulfonamide, N-(1,1-dimethylethyl)	1.00×10^5	1	400	3	9	0.66	3,660	0.004	14,600	0.0010		
10	3-nitro Isatoic anhydride	1.00×10^6	1	4,000	1	3	0.68	3,660	0.041	14,600	0.0124	91,400	0.002
11	Dimercaptothiadiazole	3.75×10^5	1	1,500	3	12	2.70	3,660	0.0156	14,600	0.005	91,400	0.0009
	Formulated to Cutting Oils	1.00×10^5	5	2,600	3	13	2.60	-					
12	Adipic acid -1,4-butanedoil - 4,4'-diphenyl methane diisocyanate	1.04×10^9	7	61,000	2	185	1.75	26,000	0.624	102,000	0.187	640,000	0.038
13	Benzyl trimethyl ammonium methoxide	2.00×10^5	1	800	3	10	1.10	3,600	0.083	14,600	0.025	91,400	0.005
14	Vitride DMTD	4.00×10^3	1	60	2	6	0.08	3,600	0.0006	14,600	0.0002	-	-
	Vitride - Cutting Oil Manufacture	1.30×10^4	1	430	2	4	0.019	-					
15	Strontium titanate	1.00×10^3	1	40	3	4	0.086	3,600	0.0004	14,600	0.0001	-	-
16	Acetone	2.00×10^9	22	115,000	1	533	0.88	81,000	1.196	321,000	0.358	2,011,000	0.073
17	Styrene Polysulfide	5.00×10^4	1	2,000	2	13	1.11	3,600	0.021	14,600	0.006	91,400	0.001
18	Hydrogenated Tallow Acids, ethanol amine condensate, ethoxylated	5.00×10^4	1	2,000	2	13	1.11	3,600	0.021	14,600	0.006	91,400	0.001
19	Surfynol 104(2,4,7,9-tetramethyl-4,7 dihydroxy-deca-5-yne)	5.00×10^3	1	200	2	17	0.25	3,600	0.0021	14,600	0.0006	91,400	0.0001
20	Allyl alcohol-Styrene Copolymer	5.00×10^5	1	2,000	1	13	1.11	3,600	0.021	14,600	0.006	91,400	0.001
21	Benzenediazonium, 2,5-dibutoxy-4-(4 morpholinyl)-sulfate	5.00×10^5	1	2,000	2	13	1.11	3,600	0.021	14,600	0.006	91,400	0.001
22	n-butylethyl-magnesium	5.00×10^5	1	2,000	3	8	1.67	3,600	0.021	14,600	0.006	91,400	0.001
23	Amberlyst Resin Catalyst	5.00×10^5	1	1,000	3	7	1.21	3,600	0.020	14,600	0.003	91,400	0.0006
24	Raney Nickel	1.00×10^6	1	2,800	3	11	1.87	3,600	0.029	14,600	0.009	91,400	0.002
25	Phosphorodithioic acid, S,S'-(thiodi-4,1,phenylene) 0,0,0',0' tetramethyl ester	5.00×10^5	1	1,390	3	12	1.43	3,600	0.014	14,600	0.004	91,400	0.0008
26	Hexachlorobenzene	1.60×10^6	10	4,500	3	149	2.11	36,000	0.047	146,000	0.014	914,000	0.003
27	Trichloroethylene	2.70×10^8	5	150,000	1	64	0.89	18,000	1.56	73,000	0.466	457,000	0.094
28	Sulfuric acid	3.00×10^{10}	160	520,000	2	6760	1.78	586,000	5.41	2,336,000	1.62	14,624,000	0.328
29	Iron (II) sulfide	5.00×10^5	2	700	1	16	0.33	7,300	0.007	29,200	0.002	182,800	0.0004
30	poly (oxy-1,2-ethane-diyl), α-phenyl-ω-hydroxy-,phosphate	5.00×10^3	7	250	3	8	0.54	3,600	0.0026	14,600	0.0008	91,400	0.0002

TABLE 11. CONSUMER DOSE FOR SAMPLE "NEW" CHEMICALS

No.	Chemical	Use	Active Popln.	Active Inhal. Dose (g)	Active Contact Dose (g)	Active Release (g)	Passive Popln.	Passive Inhal. Dose (g)	Passive Contact Dose (g)	Passive Release (g)	Disposal (g)
1	TRIS	Flame Retardant Clothes	0	--	--	--	2.2×10^{6}	0.071	2.7×10^{-4}	2.9×10^{8}	2.9×10^{8}
		Flame Retardant Rugs	0	--	--	--	6.0×10^{6}	0.55	1.6×10^{-3}	2.1×10^{8}	4.1×10^{9}
2	Benzene	Paint	1.8×10^{4}	865	48	6.7×10^{8}	1.3×10^{5}	0	0	0	0
		Adhesives	1.2×10^{5}	31	0.17	1.6×10^{8}	1.3×10^{5}	0	0	0	0
3	Asbestos	Heat Insulation	1.9×10^{5}	0.005	0	9.0×10^{6}	1.3×10^{6}	0.0004	0	9.8×10^{6}	9.3×10^{7}
		Auto Brakes	2.5×10^{6}	0.0006	0	7.2×10^{6}	2.5×10^{6}	0.025	0	3.2×10^{5}	4.5×10^{6}
		Appliances	5.0×10^{5}	<0.0002	0	1.7×10^{4}	5.0×10^{5}	2.3×10^{-5}	0	1.9×10^{4}	1.8×10^{4}
4	Ethylene Dichloride	Paint	1.9×10^{4}	216	81	1.6×10^{8}	1.3×10^{5}	0	0	0	0
		Polish	7.5×10^{4}	31-216	12	$1\text{-}6\times10^{8}$	1.3×10^{5}	0-0.14	0.08	$3\text{-}5\times10^{7}$	$0\text{-}5.3\times10^{8}$
5	Acrylonitrile	Pesticide	1.7×10^{6}	2.3	4.0×10^{-5}	1.6×10^{9}	2.5×10^{6}	1.8×10^{-9}	0	1.4×10^{4}	0
6	Benzidine Yellow	Paint	1.5×10^{5}	0.14	3.2 (5.0)	1.5×10^{7}	1.0×10^{6}	6.0×10^{-4}	0.16	1.3×10[illegible]	2.2×10[illegible]
		Ink	1.0×10^{4}	0.06	0.38	4.3×10^{5}	1.0×10^{6}	5.0×10^{-4}	0.47	4.7×10[illegible]	4.7×10^{7}
		Clothes	1000	6	0.95 (1.6)	4.3×10^{6}	1.0×10^{6}	4.5×10^{-4}	3.6	3.6×10[illegible]	5.7×10[illegible]
7	Uni Rez	Adhesive Binder	1.3×10^{5}	0.75	0.27	7.0×10^{7}	1.3×10^{5}	0.003	0.02	3.5×10^{7}	6.4×10^{8}
8	Oil of Cedarleaf	Cosmetic	2.5×10^{6}	9	0	9.2×10^{8}	2.5×10^{6}	0	0	0	0
9	2-Benzothiazole-sulfonamide		No Consumer Dose								
10	3-nitro Isatoic Acid	Chem. Int.	No Consumer Dose								
11	Vanchem DMTD	Vulcanizer	7.6×10^{6}	5.0×10^{-4}	0	3.0×10^{7}	1.5×10[illegible]	0.007	0	4.5×10[illegible]	1.0×10[illegible]
12	Adipic Acid	Dye Paint	1.8×10^{4}	0.006	8.7	5.4×10^{5}	1.3×10^{5}	0.002	0.014	3.4×10[illegible]	7.9×10[illegible]
		Dye Clothing	1.2×10^{3}	0.4	0.07	2.1×10[illegible]	1.3×10^{5}	0.0003	14	1.0×10[illegible]	4.3×10^{7}
13	Benzyltri-methylammonium methoxide	Catalyst	No Consumer Dose								
14	Vitride	Reducer	No Consumer Dose								
15	Strontium Titanate	Semi-Conductor	No Consumer Dose								
16	Acetone	Paint	1.5×10^{7}	865	144	5.2×10[illegible]	1.0×10[illegible]	0	0	2.3×10[illegible]	0
17	Styrene Polysulfide										
18	Hydrogenated Tallow Acid										
19	Surfynol	Cleaner	5.0×10^{5}	0.04	8.6	9.5×10^{7}	5.0×10^{5}	0.0003	3.3	3.9×10[illegible]	1.9×10[illegible]
20	Allyl Alcohol Copolymer	Cleaner	1.0×10^{6}	0.003	14	1.4×10^{7}	1.0×10^{6}	0.00024	1.6	4.2×10^{7}	7.5×10[illegible]
21	Benzenediazonium 2,5-Dibutoxy-4 (4-morpholynl)-Sulphate	Dye Paint	1.5×10^{5}	0.006	$6.5\times10^{-}$[illegible]	4.3×10[illegible]	1.0×10[illegible]	0.001	$6.5\times10^{-}$[illegible]	2.3×10[illegible]	6.4×10^{7}
		Dye Cloth	10^{4}	0.4	7.8×10^{-4}	1.7×10^{7}	1.0×10[illegible]	0.002	0.23	1.4×10^{7}	3.5×10[illegible]
22	n-butylethylmagnesium	Catalyst	No Consumer Dose								
23	Amberlyst	Catalyst	No Consumer Dose								
24	Raney Nickel	Catalyst	No Consumer Dose								
25	Phosphorodithioic Acid	Pesticide	1.8×10^{6}	0.035	0	7.8×10^{9}	2.5×10^{6}	0	0	0	0
26	Hexachloro-Benzene	Pesticide	7.0×10^{5}	0.71	4.8×10^{-7}	1.1×10^{9}	1.0×10[illegible]	$1.8\times10^{-7}\text{-}2.5\times10^{-6}$	0	1.0×10[illegible]	7.3×10[illegible]
27	Trichloroethylene	Paint	1.9×10^{4}	108	4.4	8.4×10^{7}	1.3×10^{5}	0	0	0	0
		Adhesive	1.3×10^{5}	28	0.004	1.5×10^{7}	1.3×10^{5}	0-0.005	0-0.001	7.6×10[illegible]	1.5×10[illegible]
		Cleaner	6.3×10^{4}	190	0.45	5.9×10^{8}	1.3×10^{5}	0	0	0	0
28	Sulfuric Acid	Eletrolyte	2.5×10^{6}	1.0×10^{-5}	1.1	3.6×10^{6}	2.5×10^{6}	8.0×10^{-4}	0	1.8×10[illegible]	1.6×10[illegible]
29	Iron Sulfide	Paint	7.5×10^{4}	0.027	2.8×10^{-4}	9.5×10^{6}	5.0×10^{5}	5.5×10^{-4}	5.5×10^{-6}	5.7×10^{7}	1.3×10[illegible]
		Electrolyte	2.5×10^{6}	1.0×10[illegible]	1.0×10^{-6}	3.6×10^{6}	2.5×10^{6}	0	0	$4.$[illegible]$\times10^{7}$	1.6×10[illegible]
30	Poly (oxy-1,2-ethane-diyl, α-phenyl-w-hydroxy-, phosphate										

APPENDIX

Table A-1. Production Volume for Various Use Functions A-1

Sources of Market Data. A-3

Table A-2. Market/Production Competitive Data by Auerbach Code . . . A-4

Table A-3. Production Volume for Chemical Function Categories. . . . A-11

B. Physical and Chemical Properties of "New" Chemicals A-15

C. Development of Diffusion Parameter. A-45

D. Chemical Permeability Parameter A-48

E. Sample Calculation for Tris - Consumer Dose A-49

TABLE A-1. PRODUCTION VOLUME FOR VARIOUS USE FUNCTIONS.

Function Code	Descriptor	Production		Sales			Annual Growth Rate %	Selling Price Range, $/lb	Number of Competitors
		Year	lb	Year	lb	Dollars			
0032	Ultraviolet Absorbers			1973$^{(2)}$	9.9x10^{6}	35x10^{6}	6-10	2.80- 10.50	11
004, 007 301 300	Accelerators, Activators, Vulcanizing Agents Polymerization Regulators	1977$^{(1)}$	152x10^{6}	1977$^{(1)}$	83.2x10^{6}	95.7x10^{6}	5	0.64-3.37	15
009				1977$^{(2)}$	4.1x10^{6}	1.4x10^{6}	6	0.17	750
014	Aerosol Propellants			1977$^{(11)}$	375x10^{6}	90x10^{6}		0.12-0.60	
049	Antifreezes			1975$^{(11)}$	218*x10^{6}	435x10^{6}	1.5-3	2.19*	7
056	Anti-Knock Agents	1977$^{(11)}$	1.35x10^{9}	1980$^{(11)}$	320x10		3		
087	Antistatic Agents			1977$^{(2)}$	4.4x10^{6}	5x10^{6}			
102	Blowing Agents			1977$^{(2)}$	355x10^{6}	167x10^{6}	9	0.47	11
102 293 296 354	Blowing Agents Oxidation Inhibitors Ozonation Inhibitors Stablizers	1977$^{(1)}$	193x10^{6}	1977$^{(1)}$	117x10^{6}	143x10^{6}	5	1.22	13
112	Catalysts			1978$^{(11)}$	1.0x10^{9}	670x10^{6}		0.67	
114	Caulking Compounds			1977$^{(2)}$	1.8x10^{9}	325x10^{6}	12	0.18	
128	Cleaners			1976$^{(2)}$		1.5x10^{9}	4		30
1330	Dyes	1977$^{(1)}$	264x10^{6}	1977	254x10^{6}	690x10^{6}	3	2.70	41
1331	Pigments (Organic)	1977$^{(1)}$	69x10^{6}	1977	57x10^{6}	268x10^{6}	6	4.66-25	35
1331	Pigments (Inorganic)			1976$^{(2)}$	2.8x10^{9}	1.3x10^{9}	9	0.40	
137	Corrosion Inhibitors			1977$^{(2)}$		1.4x10^{9}	4		10
141	Crosslinking Atents			1977$^{(2)}$	29.5x10	45x10^{6}	7	1.53	7
163	Deemulsifiers			1978$^{(11)}$	75x10^{6}		10		8
173	Detergent Builders			1977$^{(11)}$	9.8x10^{6}		3	20	
180	Antiseptics	1977$^{(1)}$	28x10^{6}	1977	11.1x10^{6}	42.2x10^{6}	1	1.39-6.40	50
186	Dryers	1977$^{(1)}$	15.4x10^{6}	1977	10.9x10^{6}	10.6x10^{6}		0.65-155	12
200	Enzymes			1977$^{(2)}$		52x10^{6}	4.5$^{(2)}$		20
206	Explosives			1976$^{(2)}$	3.3x10^{9}	450x10^{6}	6	0.14	9
211	Fertilizers			1976$^{(2)}$	97x10^{9}	6.8x10^{6}	4		33
212	Feber Forming Compounds	1977$^{(1)}$	6x10^{9}	1977	355x10^{6}	171x10^{6}		0.33-0.64	11
217	Fire Extinguishing Agents			1978$^{(11)}$	15*x10^{6}	8x10^{6}		0.53*	2
220	Flame Retardants			1977$^{(11)}$	360x10^{6}	190x10^{6}	8	0.53	40
224	Flocculating Agents			1977	60x10^{6}	5.9x10^{6}	4	0.79-1.10	
236	Fungicides	1977$^{(1)}$	143x10^{6}	1977	133x10^{6}	189x10^{6}	0	0.38-7.70	31
271	Lubricant Additives	1977$^{(1)}$	1.5x10^{6}	1977	1.3x10^{6}	492x10^{6}	10	0.26-0.73	29
272	Lubricants			1978$^{(11)}$	450x10^{6}		15		
2722	Internal Lubricants			1977$^{(2)}$	66x10^{6}	45x10^{6}	3	0.68	20
306	Plasticizers	1977$^{(1)}$	1.8x10^{9}	1977	1.7x10^{9}	632x10^{6}	6	0.28-71	54
331	Rust Inhibitors			1977$^{(11)}$	20x10^{6}				
3390	Chelating Agents	1977$^{(1)}$	168x10^{6}	1977	140x10^{6}	70x10^{6}	15	0.43-0.93	8
341	Sizes (Textile)			1977$^{(2)}$	40x10^{6}		0		
341 370	Sizes Thickeners			1977$^{(2)}$		360x10^{6}	4		
349	Soil Conditioners	1977$^{(1)}$	<236x10^{6}	1977	<219x10^{6}	<416x10^{6}	6	0.50-3.11	
3542	Heat Stabilizers			1977$^{(2)}$	94x10^{6}	80x10^{6}	2	0.85	
362	Surfactants	1977$^{(1)}$	4.7x10^{9}	1977	2.5x10^{9}	875x10^{6}	0	0.16-1.39	164
365	Tanning Agents	1977$^{(1)}$	62x10^{6}	1977	56x10^{6}	25x10^{6}	--	0.43-0.49	7
372	Toners	1977$^{(1)}$	67x10^{6}	1977	56x10^{6}	237x10^{6}	6	4.71	35
382	Water Repellents			1977$^{(2)}$		60x10^{6}	24		

*Gallons

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TABLE A-2. MARKET/PRODUCTION COMPETITIVE DATA BY AUERBACH CODE

Function Code	Function Description	Function Type* 'c'	Total No. Competitors Within Range
001	Ablatives	0.5	1-25
002	Abrasives	0.5	26-50
003	Absorbents	1	26-50
0030	Gas	1	1-25
0031	Liquid	1	1-25
0032	Ultraviolet	1	1-25
004	Accelerators	1	26-50
007	Activators	1	1-25
008	Adhesion Promotors	1	1-25
009	Adhesives	0.5	100+
012	Adsorbents	1	1-25
013	Aerating Agents	1	1-25
014	Aerosol Propellents	0.5	1-25
015	Algicides	0.5	26-50
021	Animal Repellents	0.5	1-25
029	Antiblocking Agents	1	1-25
030	Anticaking Agents	1	1-25
034	Anticracking Agents	1	1-25
035	Anticratering Agents	1	1-25
036	Anticrock Agents	1	1-25
041	Antifelting Agents	1	1-25
045	Antiflooding Agents	1	1-25
046	Antiflame Agents	1	1-25
047	Antifogging Agents	1	1-25
048	Antifouling Agents	1	1-25
049	Antifreezes	0.5	1-25
056	Antiknock Agents	1	1-25
069	Antipilling Agents	1	1-25
070	Antiplasticizers	1	1-25
071	Antiprotozoal Agents	1	1-25
0710	Amebicides	1	1-25
075	Antisagging Agents	1	1-25
076	Antiscaling Agents	1	26-50
077	Antiscorching Agents	1	1-25
079	Antiseptics	0.5	26-50
081	Antisettling Agents	1	1-25
082	Antiskid Agents	1	1-25
083	Antiskinning Agents	1	1-25
084	Antislip Finishing Agents	1	1-25
086	Antistaining Agents	1	1-25
087	Anitstatic Agents	1	26-50
088	Antitack Agents	1	26-50
096	Bactericides	1	26-50

TABLE A-2. (CONT.)

Function Code	Function Description	Function Type* 'c'	Total No. Competitors Within Range
097	Bacteriostats	1	1-25
098	Binders	1	51-100
099	Bleaches	0.5	1-25
100	Bleaching Assistants	1	1-25
101	Bloom Inhibitors	1	1-25
102	Blowing Agents	1	1-25
1020	Air Entraining Agents	1	1-25
103	Bluing Agents	1	1-25
104	Boiloff Assistants	1	1-25
105	Bright Dips	1	1-25
106	Brighteners	1	1-25
108	Carbonizing Agents	1	1-25
110	Carriers	1	1-25
1100	Dye Carriers	1	1-25
112	Catalysts	0.5	5 -100
114	Caulking Compounds	0.5	25-50
118	Chain Extenders	1	1-25
119	Chain Stoppers	1	1-25
120	Chain Transfer Agents	1	1-25
121	Chemical Intermediates	0.5	100+
1210	Inorganic	0.5	51-100
1211	Organic	0.5	51-100
1212	Polymerization	0.5	26-50
127	Clarifiers	1	1-25
128	Cleaners	0.5	26-50
129	Cloud Point Depressants	1	1-25
130	Coagulants	1	1-25
131	Coalescents	1	1-25
132	Coatings	0.5	100+
133	Coloring Agents	0.5	100+
133	Coloring Agents, Clothes	0.5	26-50
133	Coloring Agents, Paint	0.5	51-100
136	Correction Fluids	1	1-25
137	Corrosion Inhibitors	1	51-100
138	Coupling Agents	1	1-25
139	Crabbing Assistants	1	1-25
140	Creaseproofing Agents	1	26-50
141	Crosslinking Agents	1	1-25
142	Curing Agents	1	26-50
143	Currying Agents	1	1-25
144	De-inkers	1	1-25
145	Deaerating Agents	1	1-25
146	Deasphalting Agents	1	1-25

TABLE A-2. (CONT.)

Function Code	Function Description	Function Type* 'c'	Total No. Competitors Within Range
147	Dechlorinating Agents	1	1-25
1470	Antichlors	1	1-25
149	Decontaminants	1	1-25
1490	Mercury	1	1-25
1491	Poison Gas	1	1-25
1492	Radioactivity	1	1-25
150	Defoamers	1	50-100
151	Defoliants	1	1-25
153	Degreasers	0.5	1-25
154	Degummers	1	1-25
155	Dehairing Agents	1	1-25
156	Dehumidifiers	1	1-25
157	Deydrating Agents	1	1-25
158	De-icers	1	1-25
159	De-ionizers	1	1-25
160	Delignification Agents	1	1-25
161	Delustrants	1	1-25
162	Demineralizers	1	1-25
163	Demulsifiers	1	1-25
164	Denaturants	1	1-25
166	Deodorants	1	26-50
1660	Masking Agents	1	1-25
167	Depitching Agents	1	26-50
169	Descaling Agents	1	1-25
170	Desiccants	1	1-25
171	Desizing Agents	1	1-25
172	Detackifiers	1	1-25
173	Detergent Builders	1	1-25
174	Developers	1	1-25
1740	Dye Developers	1	1-25
175	Devulcanizing Agents	1	1-25
179	Discharge Printing Agents	1	1-50
180	Disinfectants	1	26-50
185	Drawing Compounds	1	1-25
186	Driers	1	1-25
187	Drilling Mud Conditioners	1	26-50
188	Drilling Muds	1	1-25
189	Dry Strength Agents	1	1-25
190	Dust Control Agents	1	1-25
191	Dusting Atents	1	26-50
192	Dye Reserving Agents	1	1-25
193	Dye Retardants	1	1-25
194	Dye Retention Aids	1	1-25
195	Electrolytes	0.5	1-25
1950	Peptizing Agents	0.5	1-25

TABLE A-2. (CONT.)

Function Code	Function Description	Function Type* 'c'	Total No. Competitors Within Range
196	Eluting Agents	1	1-25
199	Entraining Agents	1	1-25
200	Enzymes	1	26-50
205	Explosion Inhibitors	1	1-25
206	Explosives	0.5	1-25
2060	Blasting	0.5	1-25
2061	Propellant	0.5	1-25
207	Extenders	1	26-50
208	Feed Chemicals	0.5	1-25
210	Fertilizer Conditioners	1	1-25
211	Fertilizers	0.5	26-50
212	Fiber Forming Compounds	1	1-25
213	Fillers (Augmentation)	1	51-100
214	Fillers (Patching)	1	1-25
215	Filtration Aids	1	26-50
217	Fire Extinguishing Agents	1	1-25
219	Fixatives (Dye)	1	1-25
220	Flame Retardants	1	26-50
221	Flatting Agents	1	1-25
224	Flocculating Agents	1	26-50
227	Fluxes	0.5	1-25
2270	Brazing	0.5	1-25
2271	Galvanizing	0.5	1-25
2272	Soldering	0.5	1-25
2273	Tinning	0.5	1-25
2274	Welding	0.5	1-25
228	Foam Inhibitors	1	51-100
230	Formation Aids	1	1-25
232	Frothing Agents	1	1-25
233	Fuels	0.5	26-50
234	Fulling Agents	1	1-25
236	Fungicides	0.5	26-50
237	Fungistats	1	1-25
2370	Mildew Preventives	1	1-25
2371	Mold Inhibitors	1	1-25
239	Gelling Agents	1	1-25
241	Greaseproofing Agents	1	1-25
243	Heat Sealing Agents	1	1-25
244	Heat Transfer Agents	1	1-25
2440	Calefactants	1	1-25
2441	Coolants	1	1-25
2442	Refrigerants	1	1-25
248	Herbicides	0.5	26-50
250	Hunectants	1	1-25
251	Humidity Indicators	1	1-25

TABLE A-2. (CONT.)

Function Code	Function Description	Function Type* 'c'	Total No. Competitors Within Range
252	Hydraulic Fluids	0.5	1-25
2520	Automatic Transmission	0.5	1-25
256	Incendiaries	1	1-25
257	Inflating Agents	1	1-25
259	Insect Repellants	0.5	1-25
2590	Mothproofing Agents	0.5	1-25
260	Insulating Compounds	0.5	51-100
2600	Acoustical	0.5	1-25
2601	Electrical	0.5	26-50
2602	Heat	0.5	1-25
261	Intensifiers	1	1-25
2610	Dye Intensifiers	1	1-25
262	Ion Exchange Compounds	1	1-25
2623	Flotation Agents	1	1-25
263	Kier Assistants	1	1-25
264	Lachrymators	1	1-25
265	Laminating Agents	1	1-25
266	Laundry Soaps	1	1-25
269	Leveling Agents	1	1-25
2690	Dye Leveling	1	26-50
2691	Vulcanization Leveling	1	1-25
271	Lubricant Additives	1	26-50
272	Lubricants	0.5	100+
273	Markers (Textile)	1	1-25
275	Mercerizing Agents	1	1-25
276	Metal Conditioners	1	1-25
277	Microbiological Culture Media	1	1-25
278	Mordants	1	1-25
282	Nucleating Agents	1	1-25
283	Nutrients	1	1-25
2830	Bacteriological	1	1-25
284	Obscuring Agents	1	1-25
285	Odorants	1	1-25
286	Oil Repellents	1	1-25
287	Oiliness Agents	1	1-25
288	Opacifiers	1	1-25
290	Optical Brighteners	1	1-25
293	Oxidation Inhibitors	1	26-50
294	Oxidation-Reduction Indicators	1	1-25
295	Oxidizers	1	1-25
296	Ozonation Inhibitors	1	1-25
298	Pearlizing Agents	1	1-25
299	Pesticides (Fumigants)	0.5	26-50
2991	Insecticides	0.5	1-25
300	pH Control Agents	1	1-25

TABLE A-2. (CONT.)

Function Code	Function Description	Function Type* 'c'	Total No. Competitors Within Range
301	pH Indicators	1	1-25
302	Pickling Agents	0.5	1-25
304	Plastic-forming Compounds	1	26-50
305	Plasticizers	1	51-100
308	Polymerization Inhibitors	1	1-25
309	Prespotting Agents	1	1-25
310	Preservatives	1	51-100
311	Prevulcanization Inhibitors	1	1-25
312	Protective Agents	1	1-25
315	Pulping Retention Aids	1	1-25
316	Radiation Protective Agents	1	1-25
318	Reaction Media	0.5	26-50
319	Reducers	0.5	1-25
320	Refining Agents	1	1-25
322	Repulping Aids	1	1-25
323	Resists	0.5	1-25
325	Rotproofing Agents	1	1-25
327	Rubber-forming	1	26-50
328	Rubber Reclaiming Agents	1	1-25
329	Rubbing Fastness Agents	1	1-25
331	Rust Inhibitors	1	51-100
332	Rust Removers	1	26-50
333	Scavengers	1	1-25
335	Scouring Agents	1	26-50
336	Scrooping Agents	1	26-50
337	Sealants	0.5	51-100
338	Semiconductors	0.5	1-25
339	Sequestrants	1	26-50
3390	Chelating Agents	1	26-50
3391	Complexing Agents	1	1-25
340	Shrinkage Controllers	1	1-25
341	Sizes	1	26-50
342	Slime Preventives	1	1-25
344	Soaking Agents	1	1-25
345	Soap Builders	1	1-25
346	Soaping Agents	1	1-25
347	Soaping-off Assistants	1	1-25
348	Softeners	0.5	51-100
349	Soil Conditioners	0.5	1-25
350	Soil Release Agents	1	26-50
351	Soil Retardants	1	1-25
352	Solvents	0.5	100+
353	Spreading Agents	1	1-25

TABLE A-2. (CONT.)

Function Code	Function Description	Function Type* 'c'	Total No. Competitors Within Range
354	Stabilizers	1	26-50
3540	Emulsion	1	1-25
3541	Foam	1	1-25
3542	Heat	1	1-25
355	Stains	1	1-25
356	Starch Improvers	1	1-25
357	Stiffening Agents	1	1-25
358	Strippers	0.5	26-50
3580	Dye	1	1-50
3581	Paint	0.5	26-50
3582	Wax	0.5	1-25
359	Structural Binders	1	1-25
360	Structural Components	1	1-25
362	Surfactants	0.5	100+
3620	Detergents	0.5	51-100
3621	Dispersants	0.5	51-100
3622	Emulsifiers	0.5	51-100
3623	Floatation Agents	0.5	51-100
3624	Penetrants	1	51-100
3625	Rinse Aids	1	26-50
3626	Soil Suspending Agents	1	26-50
3627	Wetting Agents	1	51-100
363	Swelling Agents	1	26-50
364	Tackifiers	1	26-50
365	Tanning Agents	1	1-25
3650	Bates	1	1-25
366	Tar Removers	1	1-25
367	Tarnish Removers	1	1-25
368	Textile Conditioners	1	1-25
369	Texturizers	1	1-25
370	Thickeners	1	26-50
372	Toners	1	1-25
379	Vat Printing Assistants	1	1-25
380	Viscosity Adjustors	1	1-25
3800	Thixotropic Agents	1	1-25
3801	Viscosity Depressants	1	1-25
3802	Viscosity Improvers	1	26-50
381	Vulcanizing Agents	1	1-25
382	Water Repellents	1	26-50
383	Water Proofing Agents	1	26-50
384	Weighting Agents	1	1-25
385	Wet Strength Agents	1	1-25

*0.5 ≡ Slow-to-Penetrate Current Market
1 ≡ Quick-to-Penetrate Current Market

TABLE A-3. PRODUCTION VOLUME FOR CHEMICAL FUNCTION CATEGORIES

	Function	Annual Production, kg
2	Abrasives	4.2×10^{7} KG
2	Abrasives	
3	Absorbents	
3	Absorbents	4.2×10^{7} KG
8	Adhesion Promoters	1.8×10^{7} KG
9	Adhesives	
9	Adhesives	1.8×10^{10} KG
14	Aerosol Propellants	8.3×10^{8} KG
15	Algicides	
21	Animal Repellents	
30	Anticaking Agents	1.1×10^{8} KG
34	Anticraking Agents	5.5×10^{7}
35	Anticratering Agents	5.5×10^{7}
36	Anticrock Agents	2.6×10^{6}
41	Antifelting Agents	2.6×10^{6}
45	Antiflooding Agents	2.6×10^{8}
46	Antifume Agents	2.6×10^{6}
47	Antifogging Agents	1.0×10^{8}
48	Antifouling Agents	1.3×10^{10}
49	Antifreezes	3.7×10^{9}
56	Antiknock Agents	6.6×10^{8}
69	Antipilling Agents	2.6×10^{6}
70	Antiplasticizers	2.1×10^{9}
75	Antisagging Agents	2.9×10^{8}
77	Antiscorching Agents	8.8×10^{9}
79	Antiseptics	2.4×10^{7}
81	Antisettling Agents	5.5×10^{7}
82	Antiskid Agents	1.1×10^{9}
84	Antislip Finishing Agents	5.5×10^{8}
86	Antistaining Agents	2.2×10^{6}
87	Antistatic Agents	9.7×10^{6}
88	Antitack Agents	5.3×10^{7}
96	Bactericides	
97	Bacteriostats	1.1×10^{9}
99	Bleaches	5.5×10^{7}
102	Blowing Agents	7.9×10^{8}
103	Bluing Agents	2.2×10^{8}
106	Brighteners	3.1×10^{8}
114	Caulking Compounds	2.0×10^{6}
127	Clarifiers	1.2×10^{9}
130	Coagulants	
132	Coatings	
132	Coatings	
133	Coloring Agents	6.6×10^{7} (ink)
133	Coloring Agents	1.1×10^{9} (clothes)
133	Coloring Agents	4.4×10^{8} (paint)

TABLE A-3. (cont.)

	Function	Annual Production, kg
136	Correction Fluid	1.2x10^{7}
137	Corrosion Inhibitor	3.0x10^{8}
140	Creaseproofing Agents	6.6x10^{7}
141	Crosslinking Agents	6.6x10^{7}
142	Curing Agents	2.6x10^{9}
143	Currying Agents	1.2x10^{7}
150	Defoamers	
151	Defoliants	6.6x10^{6}
153	Degreasers	6.2x10^{8}
158	Deicers	1.3x10^{7}
161	Delustrants	6.6x10^{7}
162	Demineralizers	2.2x10^{8}
166	Deodorants	8.1x10^{8}
170	Dessicants	
171	Desizing Agents	6.6x10^{7}
173	Detergent Builders	2.0x10^{9}
174	Developers	5.5x10^{7}
180	Disinfectants	2.4x10^{7}
186	Driers	2.4x10^{7}
189	Dry Strength Agents	1.2x10^{9}
190	Dust Control Agents	
193	Dye Retardents	6.6x10^{7}
195	Electrolytes	8.8x10^{8}
200	Enzymes	2.2x10^{7}
206	Explosives	7.2x10^{9}
207	Extenders	4.3x10^{8}
210	Fertilizer Conditioners	2.2x10^{8}
211	Fertilizers	1.1x10^{10}
212	Fiber Forming Compounds	7.9x10^{8}
213	Fillers	4.2x10^{8}
214	Fillers (Patching)	4.4x10^{7}
217	Fire Extinguishing Agents	2.6x10^{8}
220	Flame Retardents	7.9x10^{8}
221	Flatting Agents	2.2x10^{8}
227	Fluxes	>2.2x10^{6}
228	Foam Inhibitors	9.9x10^{7}
230	Formation Aids	9.9x10^{7}
233	Fuels	1.0x10^{12}
236	Fungicides	
237	Fungistats	2.8x10^{8}
239	Gelling Agents	
241	Greaseproofing Agents	1.2x10^{9}
243	Heatsealing Agents	2.2x10^{7}
244	Heat Transfer Agents	2.2x10^{7}
259	Insect Repelleents	2.2x10^{7}
260	Insulating Compounds	8.8x10^{8}
261	Intensifiers	2.2x10^{7}
262	Ion Exchange Compounds	5.0x10^{7}

TABLE A-3. (cont.)

	Function	Annual Production, kg
269	Leveling Agents	7.0×10^6
271	Lubricant Additives	4.0×10^6
272	Lubricants	9.9×10^8
273	Markers (Textile)	
276	Metal Conditioners	4.4×10^7
283	Nutrient	$>2.2\times10^6$
285	Odorants	$>2.2\times10^6$
286	Oil Repellents	1.2×10^8
287	Oiliness Agents	3.2×10^6
290	Optical Brighteners	4.2×10^7
293	Oxidation Inhibitors	2.6×10^8
294	Oxidation Reduction Indicators	2.2×10^6
295	Oxidizers	
296	Ozonation Inhibitors	4.2×10^8
298	Pearlizing Agents	2.0×10^6
300	pH Control Agents	$>2.2\times10^6$
301	pH Indicators	$>2.2\times10^6$
304	Plastic Forming Compounds	4.4×10^9
305	Plasticizers	4.0×10^9
310	Preservatives	2.6×10^7
312	Protective Agetns	8.8×10^7
321	Reinforcing Agents	2.6×10^9
325	Rotproofing Agents	2.2×10^7
327	Rubber Forming Compounds	8.8×10^7
329	Rubber Fastness Agents	2.6×10^8
331	Rust Inhibitors	4.4×10^7
332	Rust Removers	1.2×10^7
335	Scouring Agents	1.2×10^8
339	Sequestrants	
340	Shrinkage Controllers	8.8×10^7
341	Sizes	
342	Slime Preventers	
345	Soap Builders	1.7×10^8
346	Soaping Agents	1.3×10^7
348	Softeners	
350	Soil Release Agents	4.0×10^6
351	Soil Retardents	4.0×10^6
352	Solvents	4.4×10^9 (paint)
352	Solvents	2.2×10^8 (adhesive)
352	Solvents	2.2×10^9 (cleaners)
354	Stabilizers	2.9×10^8
356	Starch Improvers	4.4×10^8
357	Stiffening Agents	2.6×10^8
358	Strippers	1.2×10^8
359	Structural Binders	
360	Structural Components	

TABLE A-3. (cont.)

	Function	Annual Production, kg
362	Surfactants	
362	Surfactants	6.0×10^{9}
364	Tackifiers	1.2×10^{7}
366	Tar Removers	4.4×10^{6}
367	Tarnish Removers	1.2×10^{7}
370	Thickeners	9.0×10^{8}
372	Toners	8.8×10^{7}
380	Viscosity Adjusters	
382	Water Repellents	1.4×10^{8}
383	Waterproofing Agents	6.6×10^{7}
384	Weighing Agents	4.4×10^{8}
385	Wet Strength Agents	1.2×10^{9}
	Waxes	8.8×10^{6}

B. PHYSICAL AND CHEMICAL PROPERTIES OF "NEW" CHEMICALS

CHEMICAL: Tris (2,3-dibromopropyl) phosphate

NO. 1

STRUCTURE: $(BrCH_2BrCHCH_2O)_3P = O$. $C_9H_{15}Br_6O_4P$

INFORMATION SOURCES:

1. Computer search of Chemical Abstracts
2. Personal knowledge
3. Handbook of Chemistry and Physics, 58th ed.
4. A. Leo, C. Hansch and D.E. Chin, Chem. Rev., 71, 525 (1971)
5. C. Hansch et al., J. Med. Chem., 16, 1207 (1973)
5. Chemical Use List, EPA, Federal Register, 43, 32222 (1978)
7. Aldrich Catalog, 1979

PROPERTIES: Oil, very low volatility, moderate chemical stability

Log $p^{4,5}$ (est.) = 2.53 (tripropylphosphate) + 5 (6 Br) = 7.5

m.p. °C:

Water Sol. extremely low

b.p. °C: (est.) >400

Vapor Pressure @ 20°C (est.) 10^{-5} mm Hg

Flash Pt^7 °C >112°C

d^7 2.24

USES: Flame retardant for plastic, textiles, rubber, other materials.

DIRECT TRANSPORT: Low potential for wide distribution. Steady state concentration should be:
Air: extremely low
Land: high
Water: extremely low-would sink to bottom

DIRECT SYSTEMIC UPTAKE: Capable of rapid absorption through skin and other membranes, through lungs and through walls of G.I. tract.

BY-PRODUCT FORMATION: a) Manufacture: May be produced by reaction of 2,3-dibromopropanol with phosphorous oxychloride or phosphorous pentachloride or by bromination of triallyl phosphate. Possible by-products: bis-and mono-dibromopropyl phosphate esters, bromopropenyl phosphate esters, bromopropenol, dibromopropene, allyl alcohol, hydrochloric acid, hydrobromic acid, phosphoric acid and salts. b) Processing: Possible by-products: bis-and mono-dibromopropyl phosphate esters, dibromopropanol tris-(bromopropenyl) phosphate esters, bromopropenol, dibromopropene, hydrobromic acid, phosphoric acid, tribromopropane, bromopropene.

DEGRADATION IN THE ENVIRONMENT: Subject to partial and complete hydrolysis of the phosphate ester functions, dehydrohalogenation, oxidation, and biodegradation. Also alkylating agent, capable of alkylating biomaterials (alkyl halide function).

BIO-ACCUMULATION: Not subject to bioaccumulation in the food chain. Could accumulate in the individual animal by alkylation of biopolymers.

NO. 2

CHEMICAL: Benzene

STRUCTURE:

INFORMATION SOURCES:

1. Merck Index, 9th ed., 1976
2. C. Hansch et al, J. Med. Chem., 16, 1207 (1973)
3. Personal knowledge
4. Chemical Use List, EPA, Fed. Register, 43, 32222 (1978)
5. Handbook of Chemistry and Physics
6.
7.

PROPERTIES: Liquid, volatile, chemically stable

Log P[2] = 2.13

m.p. °C:

Water Sol. 0.07%[1]

b.p. °C: 80

Vapor Pressure @ 20°C 75mm Hg

Flash Pt 10-12°C[1]

d^{15}_{4} 0.88

USES: Chemical intermediate-organic compounds. Solvent for waxes, oils, resins, etc. Reaction medium, manufacture of organic compounds, drugs, dyes, artificial leather, linoleum, airplane dopes, varnishes, lacquers. Veterinary medicine.

DIRECT TRANSPORT: Potential for wide distribution in the environment. Steady state concentrations should be Air: high
Land: intermediate
Water: low-capable of spreading on surface of water

DIRECT SYSTEMIC UPTAKE: Capable of rapid absorption through skin and other membranes, through lungs, and through walls of gastrointestinal tract.

BY-PRODUCT FORMATION:

a) Manufacture: Produced from coal during coking and cracking processes. By-Products include a variety of coal tar chemicals.

b) Processing: Relatively stable compound. Unlikely to be significant amounts of by-products formed during processing except when used as chemical intermediates.

DEGRADATION IN THE ENVIRONMENT: Subject to photochemical, oxidative and biodegradation. Initially, hydroxylated products would be formed (phenolic compounds).

BIO-ACCUMULATION: Not subject to bioaccumulation.

NO. 3

CHEMICAL: Asbestos Calcium-Magnesium Silicates (Native)

STRUCTURE:

INFORMATION SOURCES:

1. Merck Index, 9th Ed.
2. IITRI Information
3. Chemical Use List, EPA
4.
5.
6.
7.

PROPERTIES: Fine fibers, stable, non-volatile. Insoluble in water, organic solvents

m.p. °C: ______ Water Sol. Insoluble

b.p. °C: ______ Vapor Pressure @ 20°C ______

Flash Pt ______ d 2.5-3

USES: Heat insulating compound for building construction, cements, furnace and hot pipe coverings, inert filler medium, fireproof gloves, clothing, brake linings.

DIRECT TRANSPORT: Low potential for distribution. Steady state concentrations should be: Air: Low but fine dust can be suspended in air and carried by air currents, Land: High, Water: Low; again fine particles can remain suspended and carried by water currents.

DIRECT SYSTEMIC UPTAKE: Cannot be systemically absorbed through skin, lungs or intestinal walls. Can be retained embedded in lung tissue.

BY-PRODUCT FORMATION:

a) Manufacture: Obtained in mining operations. Only by-products would be associated minerals present in the mine.

b) Processing: By-products formation: negligible

DEGRADATION IN THE ENVIRONMENT: Stable (based on extensive experience, use).

BIO-ACCUMULATION: Not subject to bioaccumulation in the food chain. Could accumulate in the lungs of an individual.

NO. 4

CHEMICAL: Ethylene Dichloride

STRUCTURE: $ClCH_2CH_2Cl$ $C_2H_4Cl_2$

INFORMATION SOURCES:

1. Merck Index, 9th Ed.
2. Personal knowledge
3. A. Leo, C. Hansch and D. Elkins, Chem. Rev., 71, 525 (1971)
4. C. Hansch et al, J. Med. Chem., 16, 1207 (1973)
5. Chemical Use List, EPA
6. Handbook of Chemistry and Physics, 45th Ed.
7.

PROPERTIES: Liquid, volatile, moderate chemical stability

Log $P^{3,4}$ (estimated) = 1.54 (C_2H_5Cl) + 0.71 (Cl) = 2.25

m.p. °C:		Water Sol.	0.8%
b.p. °C:	83-84	Vapor Pressure @ 20°C	(approximate) 65mm Hg
Flash Pt	15°C	d^{20}_{4}	1.26

USES: Solvent for fuels, oils, waxes, gums, resins, rubber; solvent used in manufacture of acetyl cellulose and in tobacco extraction. Chemical intermediate.

DIRECT TRANSPORT: Potential for wide distribution in environment. Steady state concentrations should be: Air: high
Land: intermediate
Water: moderate-would tend to sink to bottom

DIRECT SYSTEMIC UPTAKE: Capable of rapid absorption through skin and other membranes, through lungs and through walls of G.I. tract.

BY-PRODUCT FORMATION:

a) Manufacture: Produced by chlorination of ethylene and by addition of hydrogen chloride to acetylene. Possible by-products; vinyl chloride, polyvinyl chloride, starting materials.

b) Processing: Possible by-products: vinyl chloride, polyvinyl chloride, hydrogen chloride, alkylated materials.

DEGRADATION IN THE ENVIRONMENT: Subject to dehydrohalogenation, oxidation, and biodegradation. Also alkylating agent of relatively low reactivity. Capable of alkylating biomaterials (alkyl balide function).

BIO-ACCUMULATION: Not subject to bioaccumulation in the food chain. Could accumulate in the individual animal by alkylation of biopolymers.

NO. 5

CHEMICAL: Acrylonitrile

STRUCTURE: $CH_2 = CH - CN$. C_3H_3N

INFORMATION SOURCES:

1. Merck Index, 9th Ed.
2. Personal knowledge
3. Handbook of Chemistry and Physics, 45th Ed.
4. Chem. Reviews, 71, 525 (1971)
5. Chemical Use List, EPA
6.
7.

PROPERTIES: liquid, volatile, unstable

Log P - 0.92

m.p. °C:

Water Sol. 7% @ 20°C

b.p. °C: 77.5

Vapor Pressure @ 20°C 87mm Hg

Flash Pt 0°C

d^{25}_{4} 0.8

USES: Chemical intermediate. Polymerization intermediate for manufacture of acrylic fibers, plastics, coatings and adhesives; modifier for natural polymers. Organic intermediate for synthesic of antioxidants, pharmaceuticals, dyes. Pesticide fumigant for grain.

DIRECT TRANSPORT:
Potential for wide distribution in the environment. Steady state concentrations should be: Air: high Land: low Water: high

DIRECT SYSTEMIC UPTAKE: Capable of rapid absorption through skin and other membrances, through lungs, and through walls of G.I. tract.

BY-PRODUCT FORMATION:

a) Manufacture: Produced by dehydration of acrylamide with phosphorouspentoxide, by addition of hydrogen cyanide to acetylene and by a special catalytic oxidation of propene. Possible by-products: starting materials, acrylic acid, acrylonitrile polymers, succinonitrile.

b) Processing: Possible by-products: hydrogen cyanide, acetylene, acrylamide, acrylic acid, polymeric materials, ammonia.

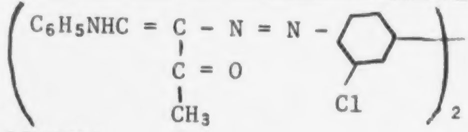
DEGRADATION IN THE ENVIRONMENT: Unstable compound. Subject to air oxidation, photochemical degradation, polymerization. loss of hydrogen cyanide, hydrolysis; sensitive to acid, alkali, readily biodegraded. Capable of alkylating biomaterials (α-β-unsaturated carbonyl compound).

BIO-ACCUMULATION: Not subject to bioaccumulation in the food chain. Could accumulate in the individual animal by alkylation of biopolymers.

CHEMICAL: Benzidine dye Benzidine yellow

NO. 6

STRUCTURE:



$C_{32}H_{26}Cl_2N_6O_4$

INFORMATION SOURCES:

1. E.A. Apps, "Printing Ink Technology," Chemical Publishing Co., NY, 1959
2. Personal knowledge
3. Chemical Use List, EPA
4.
5.
6.
7.

PROPERTIES: Solid, non-volatile, moderate chemical stability, insoluble in water

m.p. °C:

Water Sol. insoluble

b.p. °C:

Vapor Pressure @ 20°C

Flash Pt

d 1.7

USES: Pigment for use in printing inks, plastics, rubber, paint, papers, pottery, glassware, fabrics,

DIRECT TRANSPORT: Low potential for distribution in environment. Steady state concentrations should be: Air: low;fine dust could disperse in air
Land: high
Water: low; fine powder could be transported in suspension

DIRECT SYSTEMIC UPTAKE: Low potential for direct systemic absorption.

BY-PRODUCT FORMATION:

a) Manufacture: Produced by tetrazotizing 0,0-dichlorobenzidine with sodium nitrite and hydrochloric acid and reacting the tetrazonium salt with acetoacetanilide. Possible by-products: starting materials, 2,2'-dichloro-4,4'-biphenol,3,3'-dichlorobiphenyl, aniline, phenol, acetoacetic acid, nitrogen oxides.

b) Processing: Low potential for by-product formation during processing. Possible by-products: hydrolysis and cleavage products (aniline, acetic acid).

DEGRADATION IN THE ENVIRONMENT: Resistant to water, acid, alkali, resistant to heat but sensitive to photochemical degradation. Subject to oxidative and biodegradation (based on literature information and properties of functions present).

BIO-ACCUMULATION: Not subject to bioaccumulation.

NO. 7

CHEMICAL: Uni-Rez 2642

STRUCTURE:

INFORMATION SOURCES:

1. Chemical Week, March 28, 1979, p.7
2. Union Camp Literature
3. Personal Knowledge
4. Chemical Use List, EPA
5.
6.
7.

PROPERTIES: Solid resin, non-volatile, chemically stable

m.p. °C:	164	Water Sol.	Insoluble
b.p. °C:		Vapor Pressure @ 20°C	
Flash Pt		d	0.98

USES: Adhesive, binder, heat sealing agent for plastics and metals

DIRECT TRANSPORT: Extremely little potential for distribution in environment. Steady state concentration should be:
Air: essentially none
Land: high
Water: essentially none

DIRECT SYSTEMIC UPTAKE: No potential for direct systemic absorption.

BY-PRODUCT FORMATION:

a) Manufacture: No information on chemical process or composition. Presumabley, monomer starting materials (dibasic acids, alkylenediamines and/or w-amino acids could be present).

b) Processing: No information on chemical composition other than that it is a polyamide. Dibasic acids, alkylenediamines and/or w-amino acids could be by-products.

DEGRADATION IN THE ENVIRONMENT: A polyamide material would be expected to be subject to very slow hydrolytic and oxidative degradation in the environment and to slow biodegradation by microorganisms.

BIO-ACCUMULATION: Not subject to bioaccumulation.

NO. 8

CHEMICAL: Oil of Cedar Leaf

STRUCTURE: TSCA Candidate
CAS# 61789-90-2

INFORMATION SOURCES:

1. Merck Index, 9th Ed.
2. Chem. Reviews, 71, 525 (1971)
3. Personal knowledge
4. Chemical Use List, EPA
5. Computer Search, Chem. Abstracts
6.
7.

PROPERTIES: Oil, volatile, moderate chemical stability. Mixture of terpenes: α-pinene, d-thujone and α-fenchone. Estimated log P = 3.5

m.p. °C: ________

Water Sol. Practically insoluble in water

b.p. °C: 150-200

Vapor Pressure @ 20°C (approx.) 0.3-3 mm Hg

Flash Pt ________

d 0.91-0.92

USES: perfume, flavor

DIRECT TRANSPORT: Potential for moderate distribution in environment. Steady state concentrations should be: Air: moderate Land: moderate Water: low; capable of spreading on surface of water

DIRECT SYSTEMIC UPTAKE: Potential for moderately rapid absorption through skin and other membranes, through lungs and G.I. tract.

BY-PRODUCT FORMATION:

a) Manufacture: Produced by steam distillation from fresh leaves of Thuja occidentalis L., Pinaceae, a coniferous tree. Possible by-products include: other terpenes, rearrangement and oxidation products.

b) Processing: Possible by-products: rearrangement and oxidation products.

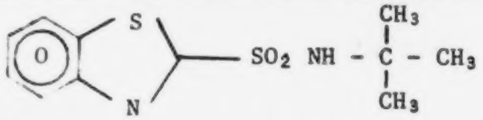
DEGRADATION IN THE ENVIRONMENT: Sensitive to light, air oxidation, subject to acid-catalyzed rearrangement, biodegradable (based on typical behavior of such aliphatic materials).

BIO-ACCUMULATION: Not subject to bioaccumulation.

NO. 9

CHEMICAL: 2-Benzothiazolesulfonamide, N-(1,1-dimethyl ethyl)

STRUCTURE:



$C_{11}H_{14}N_2O_2S_2$

INFORMATION SOURCES:

1. Computer search of Chem. Abstracts
2. Personal knowledge
3. Chem. Reviews, 71, 525 (1971)
4. J. Med. Chem., 16, 1207 (1973)
5. Handbook of Chemistry and Physics
6.
7.

PROPERTIES: Solid, extremely low volatility, moderate chemical stability.

Log P (estimated) = 2.01 (benzothiazole) + (-1.82)(SO_2NH_2) + 1.98 ($C(CH_3)_3$) = 2.2

m.p. °C: ______ Water Sol. Very slight

b.p. °C: ______ Vapor Pressure @ 20°C extremely low

Flash Pt ______ d >1

USES: Possible chemical intermediate. Possible pharmaceutical, human or veterinary use.

DIRECT TRANSPORT: Low potential for wide distribution in the environment. Steady state concentrations should be: Air: low Land: high Water: low

DIRECT SYSTEMIC UPTAKE: Capable of moderately rapid absorption by every route.

BY-PRODUCT FORMATION:

a) Manufacture: Can be prepared by oxidative chlorination of benzothiazole-2-thiol followed by treatment of the resultant benzothiazole-2-sulfonyl chloride with t-butylamine. Possible by-products include: starting materials, chlorine, acetic acid, hydrochloric acid, benzothiazole-2-sulfonyl chloride and 2-sulfonic acid.

b) Processing: Benzothiazole-2-sulfonic acid, t-butylamine

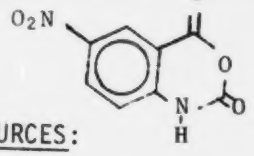
DEGRADATION IN THE ENVIRONMENT: Subject to hydrolytic, oxidative, photochemical, and biodegradation (based on presence of hydrolyzable sulfonamide function and thiazole nucleus).

BIO-ACCUMULATION: Not subject to bioaccumulation.

NO. 10

CHEMICAL: 5-Nitroisatoic Anhydride

STRUCTURE:



$C_8H_4N_2O_5$

INFORMATION SOURCES:

1. Sherwin-William Company Technical Bulletins
2. Personal knowledge
3. Chemical Use List, EPA
4. Chem. Reviews, 71, 525 (1971)
5. J. Med. Chem., 16, 1207 (1973)
6.
7.

PROPERTIES: Solid, non-volatile, moderate chemical stability

Log P (est.) = 1.15 (phthalimide) + (-0.28)(nitro) + (-0.02)(OMe) - 0.56 (Me) = 0.3

m.p. °C: 259-263 (dec.)

Water Sol. some solubility in water

b.p. °C:

Vapor Pressure @ 20°C

Flash Pt

d

USES: Chemical intermediate, organic for dyes, pharmaceuticals, etc.

DIRECT TRANSPORT: Potential for wide distribution in the environment. Steady state concentrations should be: Air: low Land: high Water: high

DIRECT SYSTEMIC UPTAKE: Potential for rapid systemic absorption by all routes.

BY-PRODUCT FORMATION:

a) Manufacture: Produced by nitration of isatoic anhydride. By-products include starting material, nitric acid, sulfuric acid, anthranilic acid, carbon dioxide, 5-nitroanthranilic acid.

b) Processing: 5-nitroanthranilic acid, carbon dioxide

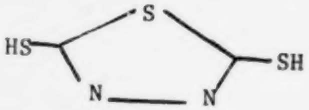
DEGRADATION IN THE ENVIRONMENT: Subject to photochemical, oxidative, hydrolytic and biodegradation (based on presence of hydrolyzable, cyclic anhydride structure and nitrobenzene ring).

BIO-ACCUMULATION: Not subject to bioaccumulation.

NO. 11

CHEMICAL: Vanchem DMTD

STRUCTURE:



$C_2H_2N_2S_3$

Dimercaptothiadiazole

INFORMATION SOURCES:

1. Vanderbilt Company Literature
2. Personal knowledge
3. Chem. Rev., 71, 525, (1971)
4. J. Med. Chem., 16, 1207 (1973)
5. Chemical Use List, EPA
6.
7.

PROPERTIES: Solid, powder, very low volatility, moderate stability

Log P (est.) = 0.44 (thiazole) + (-0.40)(pyrimidine) - 0.64 (pyridine) + 0.78 (2 SH) = 0.18

m.p. °C: 155-161

Water Sol. 3%

b.p. °C:

Vapor Pressure @ 20°C

Flash Pt

d 1.79

USES: Chemical intermediate, organic, for preparation of corrosion inhibitors, industrial organic chemicals; polymerization intermediate. Vulcanizing agent.

DIRECT TRANSPORT: Potential for moderate distribution in the environment. Steady state concentrations should be: Air: low (fine powder could form aerosols) Land: high Water: high

DIRECT SYSTEMIC UPTAKE: Potential for moderately rapid absorption through skin, walls of G.I. tract and through lungs (dust).

BY-PRODUCT FORMATION:

a) Manufacture: No information on process from company but may be produced by reaction of hydrazine with carbon disulfide or of hydrazine with phosgene and hydrogen sulfide. Possible by-products include: starting materials, nitrogen, 2,5-dihydroxy-1,3,4,-thiadiazole,2,5-dichloro-1,3,4,-thiadiazole, uncyclized adducts of hydrazine and carbon disulfide or phosgene.

b) Processing: Possible by-products include: nitrogen, hydrogen sulfide, DMTD-disulfides, hydroxythiadiazoles, carbon disulfides

DEGRADATION IN THE ENVIRONMENT: Subject to hydrolytic, oxidative and biodegradation in the environment (based on presence of sulfhydryl functions).

BIO-ACCUMULATION: Not subject to bioaccumulation.

NO. 12

CHEMICAL: Adipic Acid, 1,4-butanediol-4,4'-diphenylmethane diisocyanate

STRUCTURE: CA526375-23-5 $(C_{15}H_{10}N_2O_2 \cdot C_6H_{10}O_4 \cdot C_4H_{10}O_2)x$

INFORMATION SOURCES:

1. Computer Search Chem. Abstracts
2. Personal knowledge
3. Chemical Use List, EPA
4.
5.
6.
7.

PROPERTIES: Resin polymer, non-volatile

Moderate chemical stability

m.p. °C: ______ Water Sol. insoluble in water

b.p. °C: ______ Vapor Pressure @ 20°C ______

Flash Pt ______ d ______

USES: Coating for leather, fabrics, textiles, adhesive for leather, textiles, fiber forming compound, noncellulosic organic. Plastic forming compound, leather substitute, permeable thermoplastic elastomer, films, foils

DIRECT TRANSPORT: Low potential for wide distribution in the environment. Steady state concentrations should be: Air: essentially zero Land: high Water: essentially zero

DIRECT SYSTEMIC UPTAKE: Not subject to direct systemic uptake

BY-PRODUCT FORMATION:

a) Manufacture: Produced by heating a mixture of poly-(1,4-butanediol adipate), diphenylmethane 4,4'-diisocyanate and 1,4-butanediol. Possible by-products include: starting materials, adipic acid, 4,4'-diaminodiphenylmethane, oligomers.

b) Processing: Oligomers, adipic acid, 1,4-butanediol, 4,4'diaminodiphenylmethane

DEGRADATION IN THE ENVIRONMENT: Subject to photochemical, hydrolytic, oxidative and biodegradation (based on presence of ester fraction and aromatic rings with electron-donating substituents).

BIO-ACCUMULATION: Not subject to bioaccumulation

CHEMICAL: Benzyltrimethylammonium Methoxide

NO. 13

STRUCTURE:

C_6H_5-CH $N^+(CH_3)_3$ $\bar{O}CH_3$· $C_{10}H_{16}N \cdot CH_3O$

Supplied as 40% solution in Methanol

INFORMATION SOURCES:

1. Hexcel Specialty Chemicals Literature: Technical Data sheet, Material Safety Data Sheet, Toxicity Information
2. Personal knowledge
3. Chemical Use List, EPA
4. Chem. Reviews, 71, 525 (1971)
5. J. Med. Chem., 16, 1207 (1973)
6.
7.

PROPERTIES: Supplied as liquid solution. Compound itself would be a solid, relatively unstable, strong base, non-volatile.

m.p. °C:

Water Sol. very soluble in water

b.p. °C: (Methanol) 65

Vapor Pressure @ 20°C (Methanol) approx. 100mm Hg

Flash Pt (Methanol) 12°C

d (Solution) 0.91

Estimated Log P ($C_6H_5CH_2N^+(CH_3)_3$) = 2.13 (benezene) + (-4.15)(($(CH_2)_3$ $N^+(CH_3)_3$) - 1.02 (C_2H_5) = -3.0

USES:

Catalyst, basic, for polymerization, industrial organic chemicals.

DIRECT TRANSPORT: Strong base, would be rapidly neutralized on exposure to moist, acidic environment, carbon dioxide. Therefore, limited potential for direct transport of benzyltrimethylammonium methoxide itself. Relative steady state concentrations of the quaternary ammonium compound would be: Air: essential zero Land: moderate Water: high

DIRECT SYSTEMIC UPTAKE: Methanol would be subject to rapid absorption but the quaternary ammonium compound would undergo essentially no direct systemic absorption.

BY-PRODUCT FORMATION: a) Manufacture: Probably produced by reaction of benzyl chloride with trimethylamine followed by treatment of the product with sodium methoxide in methanol. Can also be prepared by reaction of benzylamine with excess methyl halide or dimethyl sulfate, again followed by sodium methoxide treatment. By-products indicated on the data sheet are: chloride ion, trimethylamine. Other possible by-products include: starting materials used, benzyl alcohol, benzyldimethylamine, sodium salts, benzylmethyl ether. b) Processing: Benzyl alcohol, trimethylamine, methanol, benzyldimethylamine, benzyl methyl ether.

DEGRADATION IN THE ENVIRONMENT: Methanol subject to oxidative and biodegradation. Quaternary ammonium compound thermally unstable, subject to degradation by heat, neutralization by acids, carbon dioxide, biodegradation.

BIO-ACCUMULATION: Not subject to bioaccumulation.

NO. 14

CHEMICAL: Vitride

STRUCTURE: $NaAlH_2(OCH_2CH_2OCH_3)_2$

70% solution in toluene

INFORMATION SOURCES:

1. Hexcel Specialty Chemicals Literature: Detailed Technical Bulletin; Technical Data Sheet; Material Safety and Handling Data Sheets; Toxicity Statement
2. Personal knowledge
3. Handbook of Chemistry and Physics
4. Chem. Reviews, 71, 525 (1971)
5. Chemical Use List, EPA
6.
7.

PROPERTIES: Compound itself is highly reactive, non-volatile solid. Properties of 70% solution in toluene: Strongly alkaline, non-pyrophoric. Reacts rapidly with water. Log P (toluene) = 2.69

m.p. °C:		Water Sol.	
b.p. °C:	140	Vapor Pressure @ 20°C	(est) 8mm Hg
Flash Pt	-10°C	d^{20}	1.04

USES: Reducer (chemical technology)

DIRECT TRANSPORT: Agent itself would react rapidly with moisture and therefore would not be subject to direct transport. Toluene would be subject to wide distribution in the environment. Steady state concentrations of the toluene would be: Air: moderately high Land: high Water: low

DIRECT SYSTEMIC UPTAKE: Agent again would decompose on contact with moisture in body tissues and therefore not be subject to direct systemic uptake. Toluene would be capable of rapid absorption by all routes.

BY-PRODUCT FORMATION:

a) Manufacture: Produced by reaction of sodium aluminum hydride with methoxyethanol. Possible by-products include: starting materials, sodium carbonate, sodium hydroxide, alumina.

b) Processing: Methoxyethanol, sodium carbonate, aluminum hydroxide, sodium hydroxide.

DEGRADATION IN THE ENVIRONMENT: Agent itself would be rapidly degraded on contact with moisture in environment. Toluene subject to oxidation and biodegradation.

BIO-ACCUMULATION: Not subject to bioaccumulation.

CHEMICAL: Strontium Titanate

NO. 15

STRUCTURE: $SrTiO_3$

INFORMATION SOURCES:

1. Hackh's Chemical Dictionary (1969)
2. Chemical Abstracts search
3. Personal knowledge
4. Chemical Use List, EPA
5.
6.
7.

PROPERTIES: Solid, stable, non-volatile

m.p. °C: Very high melting

Water Sol. insoluble in water

b.p. °C:

Vapor Pressure @ 20°C

Flash Pt

d

USES: Electrical insulating compounds: ceramic insulators, capacitators, resistors isulating films. Semiconductors, photoelectrodes, thermoelectric, photoelectric, optical materials, lenses, artificial gemstones, imitation diamonds

DIRECT TRANSPORT: Very low potential for wide distribution in the environment. Steady state concentrations should be: Air: essentially zero Land: high Water: essentially zero

DIRECT SYSTEMIC UPTAKE: Not subjected to significant systemic absorption.

BY-PRODUCT FORMATION:

a) Manufacture: Produced by reaction of a strontium salt (e.g., $SrCl_2$) or alkoxide with a titanium salt, titanium dioxide or titanium alkoxide. Possible by-products include: starting materials, salt metathesis products, acids, alcohols, radioactive strontium isotopes (^{90}Sr)

b) Processing: Radioactive strontium isotopes.

DEGRADATION IN THE ENVIRONMENT: Resistant to chemical and biodegradation (based on reported uses and literature information).

BIO-ACCUMULATION: Not subject to bioaccumulation.

NO. 16

CHEMICAL: Acetone

STRUCTURE:

INFORMATION SOURCES:

1. Merck Index
2. Personal knowledge
3. Handbook of Chemistry and Physics
4. Chem. Reviews, 71, 525 (1971)
5. Chemical Use List, EPA
6.
7.

PROPERTIES: Volatile liquid, moderate chemical stability

Log P[4] = -0.24

m.p. °C:

Water Sol. completely miscible with water

b.p. °C: 56.5

Vapor Pressure @ 20°C (est) 160 mm Hg

Flash Pt -20°C

d^{25} 0.788

USES: Solvent for fats, oils, waxes, resins, rubber, plastics, lacquers, varnishes, cement. Chemical intermediate, organic, industrial chemicals. Reaction medium used in manufacture of airplane dopes, rayon, photographic films, isoprene, in extraction of plant and animal substances. Stripper paint and varnish.

DIRECT TRANSPORT:

Potential for wide distribution in the environment. Steady state concentrations would be: Air: high Land: low Water: high

DIRECT SYSTEMIC UPTAKE: Capable of rapid absorption by every route.

BY-PRODUCT FORMATION:

a) Manufacture: Can be produced by: A) fermentation B) oxidation of isopropyl alcohol C) oxidative cleavage of cumene D) oxidative cracking of petroleum fraction. Possible by-products include: starting materials, butanol, peroxides, phenol, propane and other hydrocarbons, acetic acid, methanol, formaldehyde.

b) Processing: Condensation products, isopropyl alcohol, acetic acid.

DEGRADATION IN THE ENVIRONMENT: Subject to oxidative and biodegradation

BIO-ACCUMULATION: Not subject to bioaccumulation

NO. 17

CHEMICAL: Styrene polysulfide

STRUCTURE: unknown or variable composition; inadequate information for prediction of properties.

INFORMATION SOURCES:

1.
2.
3.
4.
5.
6.
7.

PROPERTIES: ____________________

m.p. °C: __________ Water Sol. __________

b.p. °C: __________ Vapor Pressure @ 20°C __________

Flash Pt[7] __________ d[7] __________

USES:

DIRECT TRANSPORT:

DIRECT SYSTEMIC UPTAKE:

BY-PRODUCT FORMATION:

a)

b)

DEGRADATION IN THE ENVIRONMENT:

BIO-ACCUMULATION:

NO. 18

CHEMICAL: Hydrogenated tallow acids; condensate, ethoxylated

STRUCTURE: unknown or variable composition; inadequate information for prediction of properties.

INFORMATION SOURCES:

1.
2.
3.
4.
5.
6.
7.

PROPERTIES:

m.p. °C:

Water Sol.

b.p. °C:

Vapor Pressure @ 20°C

Flash Pt[7]

d[7]

USES:

DIRECT TRANSPORT:

DIRECT SYSTEMIC UPTAKE:

BY-PRODUCT FORMATION:

a)

b)

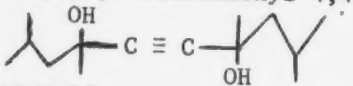
DEGRADATION IN THE ENVIRONMENT:

BIO-ACCUMULATION:

NO. 19

CHEMICAL: Surfynol 104

STRUCTURE: 2,4,7,9-tetramethyl-4,4-dihydroxydeca-5-yne



$C_{14}H_{26}O_2$

INFORMATION SOURCES:

1. Air Products and Chemicals Technical Bulletin
2. Personal knowledge
3. Chem. Reviews, 71, 525 (1971)
4. J. Med. Chem., 16, 1207 (1973)
5. Chemical Use List, EPA
6.
7.

PROPERTIES: Waxy solid, moderate chemical stability, non-volatile

Log P (est.) = 1.27 (decamethyleneglycol) + 0.4 (C ≡ CH) -1.02 (C_2H_5) + 2.24 ($4CH_3$) = 2.9

m.p. °C: 37

Water Sol. 0.1%

b.p. °C:

Vapor Pressure @ 20°C

Flash Pt

d 0.89

USES: Surfactant, defoaming, nonionic, defoamer, detergent, cleaning metal surfaces. Dispersant, wetting agent for water-based coatings, inks, pigments, and paints.

DIRECT TRANSPORT: Intermediate potential for wide distribution in the environment. Steady state concentrations should be: Air: low Water: moderate Land: high

DIRECT SYSTEMIC UPTAKE: Capable of rapid systemic absorption by all routes.

BY-PRODUCT FORMATION:

a) Manufacture: Produced by reaction of sodium acetylide with methyl isobutyl ketone. Possible by-products include: starting materials, sodium hydroxide, ethynylisobutylmethylcarbinol, acetylene.

b) Processing: By-products not likely to form during processing but possible ones include: tetramethyl-5-oxodecanediol, ethynylisobutylmethylcarbinol, methylisobutyl ketone.

DEGRADATION IN THE ENVIRONMENT: Subject to oxidative, alkaline and biodegradation in the environment. (Based on presence of acetylenic function and adjacent hydroxyl substituents.)

BIO-ACCUMULATION: Not subject to bioaccumulation.

NO. 20

CHEMICAL: Allyl Alcohol Styrene Copolymer CAS 25119-62-4

STRUCTURE: $(C_8H_8\cdot C_3H_6O)x$

INFORMATION SOURCES:

1. Computer search Chem. Abstracts
2. Personal knowledge
3. Chemical Use List, EPA
4.
5.
6.
7.

PROPERTIES: Resin polymer, non-volatile, moderate chemical stability

m.p. °C:

Water Sol. insoluble

b.p. °C:

Vapor Pressure @ 20°C

Flash Pt

d

USES: Coating component, lithographic offset printing plates, electrodeposition, etc. Plastic forming compound. Filler (augmentation) for printing inks. Cleaning compositions, dental plates.

DIRECT TRANSPORT: Low potential for wide distribution in the environment. Steady state concentrations sould be: Air: essentiall zero Land: high Water: essentially zero

DIRECT SYSTEMIC UPTAKE: Not subject to direct systemic uptake.

BY-PRODUCT FORMATION:

a) Manufacture: Produced by radical copolymerization of styrene and allyl alcohol. Possible by-products include monomers, oligomers, traces of radical initiator and its reduction product(s) (e.g., t-butyl hydroperoxide, t-butyl alcohol, propanethiol, dipropyl disulfide.

b) Processing: Oligomeric breakdown products.

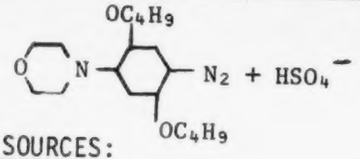
DEGRADATION IN THE ENVIRONMENT: Subject to photochemical, oxidative, thermal and biodegradation. (Based on presence of aliphatic alcohol groups, alkyl-substituted benzene rings.)

BIO-ACCUMULATION: Not subject to bioaccumulation.

NO. 21

CHEMICAL: Benzenediazonium, 2,5-dibutoxy-4-(4-morpholinyl)-sulfate (1:1)

STRUCTURE:



$C_{18}H_{34}N_3O_3 \cdot HSO_4$

INFORMATION SOURCES:

1. Computer search of Chem. Abstracts
2. Personal knowledge
3.
4.
5.
6.
7.

PROPERTIES: Thermally unstable solid, non-volatile, photosensitive

m.p. °C:

Water Sol. soluble

b.p. °C:

Vapor Pressure @ 20°C

Flash Pt

d

USES: Dyes, nonsilver halide photo films, diazo process masters

DIRECT TRANSPORT: Sensitive to light and heat. Little or no chance for wide distribution by direct transport.

DIRECT SYSTEMIC UPTAKE: Highly polar. Little or no potential for direct systemic absorption.

BY-PRODUCT FORMATION:

a) Manufacture: Produced by treatment of 2,5-dibutoxy-4-(4-morpholinyl)-aniline with sodium nitrite and sulfuric acid. Possible by-products include: starting materials, nitrogen, nitrogen oxides, dibutoxymorpholinylphenol, dibutoxymorpholinylbenzene, sodium hydrogen sulfate, N-nitrosomorpholine.

b) Processing: Corresponding azo dye, substituted phenol, benzene.

DEGRADATION IN THE ENVIRONMENT: Will be rapidly degraded by light and heat.

BIO-ACCUMULATION: No potential for bioaccumulation.

NO. 22

CHEMICAL: n-Butylethylmagnesium (BEM)

STRUCTURE: Supplied as 10-15% solution in heptane.

INFORMATION SOURCES:

1. Stauffer Chemicals Technical Bulletin
2. Personal knowledge
3. Handbook of Chemistry and Physics
4. Chem. Reviews, 71, 525 (1971)
5. J. Med. Chem., 16, 1207 (1973)
6. Chemical Use List, EPA
7.

PROPERTIES: Reagent unstable, waxy solid, reacts explosively with water, pyrophoric. Solution in heptane, non-pyrophoric liquid but reacts vigorously with water and air.

m.p. °C: ____________ Water Sol. Heptane insoluble in water

b.p. °C: (n-heptane) 98.4 Vapor Pressure @ 20°C (heptane) 10mm Hg

Flash Pt (heptane) -1°C d (solution) 0.7 @ 30°C

Solution contains small amounts of Al and Cl. Log P (heptane, est.): 2.41 (heptanol) + 0.56 (methyl) - (-1.03)(CH_2OH) = 4

USES:

Catalyst for formation of plastics and rubber materials, olefin polymerization, synthetics. Industrial organic chemicals.

DIRECT TRANSPORT: BEM would be rapidly decomposed and would not be subject to direct transport in the environment. Heptane solvent would be subject to wide distribution. Steady state concentrations should be: Air: high Land: moderately high Water: low.

DIRECT SYSTEMIC UPTAKE: BEM would react vigorously with biological tissue, be decomposed, and would not be subject to direct absorption. Heptane solvent would be rapidly absorbed by all routes.

BY-PRODUCT FORMATION:

a) Manufacture: May be produced by reaction of butyl and ethyl chlorides with magnesium or of the corresponding alkyl lithium reagents with magnesium chloride. By-products may include starting materials, lithium chloride, butane, ethane, butene, ethylene, butanol, ethanol.

b) Processing: Butane, ethane, magnesium oxide, butene, ethylene, butanol, ethanol, magnesium alkoxides.

DEGRADATION IN THE ENVIRONMENT: BEM subject to rapid decomposition by air and moisture. Heptane subject to oxidative and biodegradation.

BIO-ACCUMULATION: Not subject to bioaccumulation.

NO. 23

CHEMICAL: Amberlyst 15

STRUCTJRE: Synthetic resin catalyst

INFORMATION SOURCES:

1. Rohm and Haas Technical Bulletin
2. Personal knowledge
3. U.S. Pharamacopeia (1970)
4.
5.
6.
7.

PROPERTIES: Sulfonic acid resin. Solid, bead form, strongly acidic resin, non-volatile, stable. Particle size approximately 95% in the range 0.3-0.8 mm diam.

m.p. °C:		Water Sol.	insoluble
b.p. °C:		Vapor Pressure @ 20°C	
Flash Pt		d	0.6

USES: Catalyst, industrial organic chemicals, polymerization of olefins to form rubbers.

DIRECT TRANSPORT: Little potential for direct transport. Steady state concentrations should be: Air: essentially zero Land: high Water: essentially zero.

DIRECT SYSTEMIC UPTAKE: No potential for direct systemic absorption.

BY-PRODUCT FORMATION:

a) Manufacture: No information as to chemical composition other than that material is a sulfonic acid polymeric resin. Therefore, can say little about manufacturing process or possible by-products. May be prepared by sulfonation of a polymer or by polymerization of an unsaturates sulfonic acid derivative. Possible by-products would be monomers, oligomers, sulfuric acid.

b) Processing: Possible formation of sulfur trioxide, sulfuric acid.

DEGRADATION IN THE ENVIRONMENT: Resistant to environmental degradation. May be somewhat susceptible to oxidative and thermal degradation. (Based on information from manufacture.)

BIO-ACCUMULATION: No potential for bioaccumulation.

NO. 24

CHEMICAL: Raney Nickel

STRUCTURE:

INFORMATION SOURCES:

1. Merck Index
2. L.F. Feiser and M. Feiser, "Reagents for Organic Synthesis," John Wiley & Sons, NY, 1967.
3. Personal knowldege
4. Chemical Use List, EPA
5. Handbook of Chemistry and Physics
6.
7.

PROPERTIES: Pyrophoric; supplied as 50:50 alloy with aluminum or covered with solvent, generally water or ethanol. Solid, non-volatile powder. Dissolves in acid with release of hydrogen.

m.p. °C:

Water Sol. insoluble

b.p. °C: 2,730

Vapor Pressure @ 20°C

Flash Pt

d >1

USES: Catalyst, hydrogenation of organic chemicals.

DIRECT TRANSPORT: Catalyst, when released from alloy with aluminum and not covered with solvent, ignites spontaneously in air and is converted to nickel oxides. Therefore, essentially no potential for direct transport.

DIRECT SYSTEMIC UPTAKE: Essentially no potential for direct systemic uptake.

BY-PRODUCT FORMATION:

a) Manufacture: Produced by fusing 50 parts nickel with 50 parts aluminum, pulverizing the alloy and dissolving out most of the aluminum with aqueous sodium hydroxide. By-products include aluminum, sodium hydroxide aluminum hydroxide, nickel oxides.

b) Processing: Aluminum, aluminum hydroxide, nickel oxides, nickel salts.

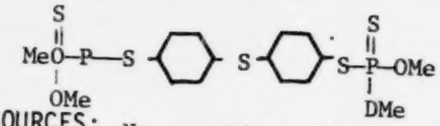
DEGRADATION IN THE ENVIRONMENT: Rapidly converted to nickel oxides, nickel salts in the reactions with air, acids.

BIO-ACCUMULATION: Not subject to direct accumulation. Nickel salts, oxides, could conceivably be accumulated.

CHEMICAL: Phosphorodithioic acid, S,S'-(thiodi-4,1-phenylene) tetramethyl ester

NO. 25

STRUCTURE:



$C_{16}H_{20}O_4S_5$

INFORMATION SOURCES: No specific information on compound available

1. Personal knowledge
2.
3.
4.
5.
6.
7.

PROPERTIES: Solid, non-volatile

m.p. °C:

Water Sol. insoluble

b.p. °C:

Vapor Pressure @ 20°C

Flash Pt

d

USES: Insecticide, pesticide

DIRECT TRANSPORT: Low potential for wide distribution in the environment. Steady state concentration should be: Air: very low Land: high Water: very low

DIRECT SYSTEMIC UPTAKE: Capable of slow absorption by all routes.

BY-PRODUCT FORMATION:

a) Manufacture: May be produced by reaction of dimethyl chlorothiophosphate with bis(4-mercaptophenyl) sulfude in the presence of alkali. Possible by-products include: starting materials, disulfides, methyl thiophosphoric acid, sodium chloride.

b) Processing: Phosphoric acid derivatives, bis-(4-mercaptophenyl) sulfide and disulfides.

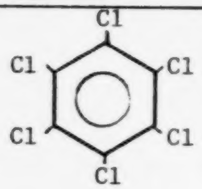
DEGRADATION IN THE ENVIRONMENT: Subject to photochemical thermal, hydrolytic and biodegradation. (Based on presence of phosphatiester functions and sulfur-containing groups.)

BIO-ACCUMULATION: Not subject to bioaccumulation in the food chain.

NO. 26

CHEMICAL: Hexachlorobenzene

STRUCTURE:



C_6Cl_6

INFORMATION SOURCES:

1. Merck Index
2. Personal knowledge
3. Handbook of Chemistry and Physics
4. Chem. Review, 71, 525 (1971)
5. J. Med. Chem. 16, 1207 (1973)
6. Chemical Use List, EPA
7.

PROPERTIES: Solid, low volatility, very stable

Log P (estimated) = 2.13 (benzene) + 4.26 (6Cl) = 6.4

m.p. °C: 231 Water Sol. extremely low

b.p. °C: 323-326 Vapor Pressure @ 20°C (est.) 10^{-3}mm Hg

Flash Pt ______ d 2.04

USES: Chemical intermediate, organic, fungicide

DIRECT TRANSPORT: Low potential for wide distribution in environment. Steady state concentrations could be: Air: low Land: high Water: low

DIRECT SYSTEMIC UPTAKE: Capable of slow absorption through skin and other membrane lungs and walls of G.I. tract.

BY-PRODUCT FORMATION:

a) Manufacture: May be produced by perchlorination of benzene in the presence of iron catalyst. By-products may include: iron salts, benzene, chlorine, lower chlorobenzene homologs, hydrogen chloride, benzene hexachloride.

b) Processing: By-products may include lower chlorbenzenes homologs.

DEGRADATION IN THE ENVIRONMENT: Resistant to chemical and biodegradation. Subject to photochemical degradation and degradation by alkali. (Perhalogenated aromatic.)

BIO-ACCUMULATION: High potential for bioaccumulation.

NO. 27

CHEMICAL: Trichloroethylene

STRUCTURE: $Cl_2C = CHCl$

INFORMATION SOURCES:

1. Merck Index
2. Personal knowledge
3. Chem. Review, 71, 525 (1971)
4. J. Med. Chem., 16, 1207 (1973)
5. Chemical Use List, EPA
6.
7.

PROPERTIES: Liquid, nonflammable, moderate stability
Log P (estimated) = 1.54 (ethyl chloride) + 1.42 (2 Cl) + 0.17 (allyl alcohol) - (+0.34) (propyl alcohol) = 2.8

m.p. °C: ______ Water Sol. practically insoluble in water

b.p. °C: 86.7 Vapor Pressure @ 20°C 60 mm Hg

Flash Pt ______ d^{20} 1.46

USES: Solvent for fats, oils, waxes, resins, rubber, paints, varnishes, cellulose esters and ethers. Solvent for dry cleaning, solvent for extraction, industrial chemical intermediate, organic, reaction medium, stripper, degreasing.

DIRECT TRANSPORT: Potential for wide distribution in the environment. Steady state concentrations should be: Air: high Land: intermediate Water: low

DIRECT SYSTEMIC UPTAKE: Capable of rapid absorption by every route.

BY-PRODUCT FORMATION:

a) Manufacture: Produced by dehydrohalogenation of tetrachloroethane. Possible by-products include: starting material, calcium carbonate, calcium chloride, hydrochloric acid, dichloroacetylene, glyoxal, oxalic acid, chloroacetic acid.

b) Processing: Hydrochloric acid, dichloroacetylene, oxalic acid, chloracetic acid, glyoxal.

DEGRADATION IN THE ENVIRONMENT: Slowly decomposed by light in the presence of moisture. Also subject to degradation by heat, alkali, air oxidation. Relatively resistant to biodegradation. (Olefinic function stabilized by polychloro nibrtitution.)

BIO-ACCUMULATION: Significant potential for bioaccumulation.

NO. 28

CHEMICAL: Sulfuric Acid

STRUCTURE:

INFORMATION SOURCES:

1. Merck Index
2. Personal knowledge
3. Handbook of Chemistry and Physics
4. Chemical Use List, EPA
5.
6.
7.

PROPERTIES: Corrosive, oily liquid, hygroscopic, moderate stability

m.p. °C:

Water Sol. Miscible with water

b.p. °C: 330 (approx.)

Vapor Pressure @ 20°C (est.) 2×10^{-4} mm Hg

Flash Pt

d 1.84

USES: Reaction medium, inorganic reagent chemical used in manufacture of fertilizers explosives, dystuffs, other acids, parchment, paper, glue, purification of petroluem, etc., pickling agent

DIRECT TRANSPORT: Highly reactive compound; undiluted acid will dehydrate and/or oxidize the majority of materials with which it comes in contact. Potential for relatively wide distribution of unreacted acid. Steady state concentrations should be: Air: low (can form aerosols) Land: low Water: high

DIRECT SYSTEMIC UPTAKE: Undiluted acid will char tissues with which it comes in contact. Diluted acid can be absorbed by all routes.

BY-PRODUCT FORMATION:

a) Manufacture: Produced by the oxidation of sulfur dioxide (e.g., with oxygen and nitric oxide) followed by hydration of the resultant sulfur trioxide. Possible by-products include: starting materials. sulfurous acid, nitrogen dioxide, sulfur trioxide, water.

b) Processing: Sulfur trioxide, sulfur dioxide, sulfurous acid, water.

DEGRADATION IN THE ENVIRONMENT: Will be diluted by absorption of water from its surroundings and reduced on contact with materials that can be oxidized; neutralized by basic substances, can enter into metabolic processes.

BIO-ACCUMULATION: Not subject to bioaccumulation.

NO. 29

CHEMICAL: Iron (II) Sulfide FeS

STRUCTURE:

INFORMATION SOURCES:

1. Merck Index
2. Personal knowledge
3. Handbook of Chemistry and Physics
4. Chemical Use List, EPA
5.
6.
7.

PROPERTIES: Solid, non-volatile, moderate chemical stability.

m.p. °C: 1194

Water Sol. $6 \times 10^{-4}\%$

b.p. °C:

Vapor Pressure @ 20°C

Flash Pt

d 4.84

USES: Inorganic chemical reagent used in the laboratory. Stain for ceramics, pigment for paints, lubricant coating, electrode material.

DIRECT TRANSPORT: Low potential for direct transport. Steady state concentrations should be: Air: essentially zero (except when aerosolized); Land: high Water: extremely low

DIRECT SYSTEMIC UPTAKE: Essentially no potential for direct systemic uptake

BY-PRODUCT FORMATION:

a) Manufacture: Produced by reaction of iron with sulfur. Also available as the natural mineral. Possible by-products include: starting materials, hydrogen sulfide, iron oxides.

b) Processing: Sulfur, iron oxides, hydrogen sulfide.

DEGRADATION IN THE ENVIRONMENT: Subject to oxidative degradation by moist air, decomposition by acids; biodegradation by microorganisms. (Based on literature information.)

BIO-ACCUMULATION: Not subject to bioaccumulation.

CHEMICAL: poly (oxy-1,2-ethane-diyl) α-phenyl-ω-hydroxy-, phosphate NO. 30

STRUCTURE:

Unknown or variable composition, inadequate information for prediction of properties.

INFORMATION SOURCES:

1.
2.
3.
4.
5.
6.
7.

PROPERTIES:

m.p. °C:		Water Sol.	
b.p. °C:		Vapor Pressure @ 20°C	
Flash Pt		d	

USES:

DIRECT TRANSPORT:

DIRECT SYSTEMIC UPTAKE:

BY-PRODUCT FORMATION:

a)

b)

DEGRADATION IN THE ENVIRONMENT:

BIO-ACCUMULATION:

C. DEVELOPMENT OF DIFFUSION PARAMETER

The release:

$$\frac{dn}{dt} = D\nabla^2 n$$

n = parts/cm^3
D = cm^2/sec

At equilibrium,

$$\frac{dn}{dt} \rightarrow 0,$$

For 1-dimensional problem, $\nabla^2 \longrightarrow \frac{\partial^2}{\partial Z^2}$

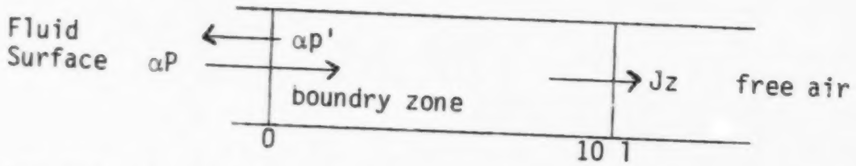
$$\frac{\partial^2 n}{\partial^2 Z} = 0$$

$$n = AZ + B$$

$$J_z = -D\,\frac{\partial n}{\partial Z} \qquad (1)$$

Suppose that $n \sim 0$ (i.e. removed by convective processes) at a distance (Z') of about 10 l from the surface (l = mean free path, 3×10^{-5} cm in air). Then

$$0 \sim AZ' + B \text{ or } A = -B/Z' \qquad (2)$$



The rate at which molecules escape from the fluid surface due to a finite vapor pressure is

$$\Phi = \frac{P}{\sqrt{2\pi mkT}} = \alpha P,$$

where P = the vapor pressure (dyne/cm^2)

m = the particle mass (g)

kT = the thermal energy per particle (ergs)

Φ = the flux outward (particles/cm^2 sec)

However, the effective rate at which evaporation occurs is usually smaller than this number because of back diffusion. For a closed system, at equilibrium, the backward flow equals the outward flow (e.g. Φ). For an open system, some material would carry away sufficient heat as to cause the liquid to freeze (i.e. like blowing very hard on hot soup). The condition at the boundary zone is:

$$\alpha P = \alpha P' - D\frac{\partial n}{\partial Z}$$

where P' is the partial pressure of the vapor phase in the boundary zone and is equal to

$$P' = \frac{nRT}{N_o}$$

where N_o = Avogadro's number - 6.023×10^{23} particles/mole

N = the particle density (number/cm^3)

R = the gas constant 8.64×10^6 ergs/°K mole

T = the absolute temperature (°K)

This constraint is thus:

$$\alpha P = \frac{\alpha nRT}{N_o} - D\frac{\partial n}{\partial Z}$$

Using (1) - evaluated at $Z = 0$

$$\alpha P = \frac{\alpha RT}{N_o} B - DA$$

Using (2)

$$\alpha P = \frac{\alpha RT}{N_o} B + \frac{DB}{Z'} = B\left(\frac{\alpha RT}{N_o} + \frac{D}{Z'}\right)$$

$$B = \frac{\alpha P}{\frac{\alpha RT}{N_o} + \frac{D}{Z'}}, \quad A = \frac{-\alpha P}{\frac{\alpha RTZ'}{N_o} + D}$$

But $J_z' - -D\frac{\partial n}{\partial Z} = \frac{D\alpha P}{\frac{\alpha RTZ'}{N_o} + D}$ is the rate at which material leaves the surface (particle/cm^2 sec)

So

$$Jz = \frac{D\alpha P\ \rho^{-1} Mw\ C}{\alpha RTZ' + N_o D}$$

is the rate of boil off in the units (cm/sec) from a mixture containing percent of the chemical of density ρ, (g/cc) and molecular weight Mw.

Thus, the time required for 50% the material in a film to be released (assuming no surface retardation) is:

$$t_{\frac{1}{2}} \text{ release} \simeq y/(2J_z)$$

where y = the thickness of the film (cm)

$$t_{\frac{1}{2}} \text{ release} \simeq \frac{\rho y(\alpha RTZ' + N_o\ D)}{D\ \alpha\ P\ \ Mw\ C}$$

Note that $t_{\frac{1}{2}}$ approaches zero as D and P become larger. For room temperature substances:

$$a \simeq 6 \times 10^{16}\ (Mw)^{-2}$$

$$D \quad \frac{2}{3\sqrt{\pi}\ \rho\ \delta_o} \ \frac{(kT)^3}{m} \simeq 0.185\ \frac{cm}{sec} \text{ for } N_2, \quad Z' \sim 5 \text{ cm}$$

D. CHEMICAL PERMEABILITY PARAMETER

The defining equation for the chemical permeability (P) of a membrane with respect to a given chemical at concentration C_o on one side of it and C_1 on the other side of it is:

$$P = \frac{V}{At} \ln \frac{C_o}{C_o - C_1}$$

where V = the volume containing C_1

A = membrane area

t = time

P is constant for times t long enough to go beyond transient conditions. For human skin and various chemicals, this time appears to be about 30 minutes.

If $C_1 << C_o$, then

$$p = \frac{V}{At} \; - \ln \left(1 - \frac{C_1}{C_o}\right. \sim \frac{V\ C_1}{At\ C_o} = \frac{\text{molar dose}}{Atc_o}$$

or

mass dose = $AtC_oP\ MW$

Now, the value of P can be estimated from the data of Treherne, and others, in terms of the partition coefficient (Pi) of the chemical, its molecular weight and solubility. The relationship is:

$$P \sim \text{Beta} \cdot \sqrt{\text{Sol}/\text{MW}} \cdot 10^{-0.6|\log \text{Pi}|}$$

where Beta $\sim 10^{-3}$

Discussion of relations of this type is in Idson. Using this value,

mass dose = $AtC_o \; \sqrt{\text{Sol MW}} \; 10^{-(4+0.6|\log \text{Pi}|)}$, for A ($m^2$), t (min), C_o (moles/liter, Sol (mass fraction) and MW (AMU).

E. Sample Calculation for Tris - Consumer Dose

```
RUN EXPOSE
STANDARD SETUP (0) OR SPECIAL (1)
? 0
INPUT THE NAME OF THE CHEMICAL TO BE EVALUATED
? TRIS
INPUT THE VAPOR PRESSURE (MM HG) FOR TRIS.
? 1E-5
INPUT THE MOLECULAR WEIGHT OF TRIS.
? 297
INPUT THE DENSITY (G/CC) OF TRIS
? 2.24
INPUT WATER SOLUBILITY (0 - 1)
? 1E-4



INPUT PARTITION COEFFICIENT - IF UNKNOWN, ENTER 1
? 7.5\5.7\4E7
INPUT THE NAME OF THE EPA FUNCTION CATEGORY
? FLAMERETARDENT
INPUT MARKET SHARE ESTIMATE (0 - 1) FOR TRIS IN EPA
FUNCTION CATEGORY FLAMERETARDENT.
? .03

   INPUT TOTAL SHIPMENTS (KG) FOR ALL CHEMICALS IN THE
CATEGORY FLAMERETARDENT.
? 1.6E8
INPUT THE NAMES OF THE EPA USE CATEGORIES
RELEVANT TO FLAMERETARDENT (I.E. TRIS) -- (ENTER -1 TO STOP)
? CLOTHES
INPUT THE NAMES OF THE EPA USE CATEGORIES
RELEVANT TO FLAMERETARDENT (I.E. TRIS) -- (ENTER -1 TO STOP)
? RUGS
INPUT THE NAMES OF THE EPA USE CATEGORIES
RELEVANT TO FLAMERETARDENT (I.E. TRIS) -- (ENTER -1 TO STOP)
? -1
INPUT THE FRACTION (0.0 - 1.0) OF TRIS ESTIMATED
TO BE PRODUCED THAT WOULD BE USED IN PRODUCTS IN THE
EPA USE CATEGORY - CLOTHES.
? .1
INPUT % COMPOSITION OF PRODUCT THAT TRIS MAKES UP.
? .03
INPUT ACTIVE POPULATION (0 TO 1) FOR CLOTHES
? .000
INPUT PASSIVE POPULATION (0 TO 1) FOR CLOTHES
? 1
INPUT POPULATION LOADING FACTORS FOR ACTIVE AND PASSIVE PHASES


? 1,.5
INPUT THE FRACTION (0 TO 1) OF PRODUCTS IN THE
CATEGORY CLOTHES THAT CONTAIN FLAMERETARDENT
? 1
INPUT THE THICKNESS OF THE RELEVANT LAYER (CM)
FROM THE USE TABLE.
? .05
```

(cont.)

```
INPUT THE MINIMUM AND MAXIMUM VALUES FOR THE
EFFECTIVE DIFFUSIVITY AND/OR ABSORPTIVITY
WITHIN THE MATERIAL (0 TO 1).
(NOTE - 1 MEANS MAXIMUM VOLATILE RELEASE AND 0 MEANS NO RELEASE
? .2,.2
INPUT CONTACT FACTORS FOR THE ACTIVE AND PASSIVE
STAGES - (0 TO 1) WHERE 1 IS MAXIMUM CONTACT.
? 1,1
INPUT CONTACT DURATION FACTORS FOR THE ACTIVE AND PASSIVE

? 1,60000
INPUT SKIN AREA IN CONTACT WITH THE CHEMICAL DURING
THE ACTIVE AND PASSIVE EXPOSURE PERIODS - (0 TO 1)
WHERE 1 REFLECTS WHOLE BODY EXPOSURE.
? .1,.8
INPUT THE FRACTION OF THE MATERIAL ACTUALLY IN CONTACT
IN CONTACT WITH THE SKIN AT ANY GIVEN TIME FOR THE
ACTIVE AND PASSIVE STAGES (0 TO 1).
? .1,.5
INPUT THE FRACTIONS OF SOLID LOST DURING THE ACTIVE,
PASSIVE AND PASSIVE-BYPASS STAGES OF ACTIVITY (0.0 TO 1.0)
? .02,.5,.48
INPUT THE CHARACTERISTIC EXPOSURE TIMES FOR THE
ACTIVE AND PASSIVE STAGES OF PRODUCT USE (HRS).
? 0,800
INPUT THE EFFECTIVE DILUTION VOLUMES FOR THE ACTIVE
AND PASSIVE STAGES OF PRODUCT USE (M CUBED).
? 40,40

POPULATION      DOSE(KG)        TREL(SEC)      T-ACT(SEC)      T-PASS(SEC)
 0              0               2.45587E+08    0               2.88000E+06


 1              0               0
 2              .0191235        2.86852E+06
 3              0               9.60000E+06
 4              .388542         1.20870E+08
 5              0               3.46662E+08
INPUT THE FRACTION (0.0 - 1.0) OF TRIS ESTIMATED
TO BE PRODUCED THAT WOULD BE USED IN PRODUCTS IN THE
EPA USE CATEGORY - RUGS.
? .9
INPUT % COMPOSITION OF PRODUCT THAT TRIS MAKES UP.
? .3
INPUT ACTIVE POPULATION (0 TO 1) FOR RUGS
? 0
INPUT PASSIVE POPULATION (0 TO 1) FOR RUGS
? 1
INPUT THE POPULATION LOADING FACTORS FOR THE
ACTIVE AND PASSIVE STAGES
? 1,.4
INPUT THE FRACTION (0 TO 1) OF PRODUCTS IN THE
CATEGORY RUGS THAT CONTAIN FLAMERETARDENT
? 1
```

(cont.)

```
INPUT THE THICKNESS OF THE RELEVANT LAYER (CM) :
FROM THE USE TABLE.
? .05
INPUT THE MINIMUM AND MAXIMUM VALUES FOR THE
EFFECTIVE DIFFUSIVITY AND/OR ABSORPTIVITY
WITHIN THE MATERIAL (0 TO 1).
(NOTE - 1 MEANS MAXIMUM VOLATILE RELEASE AND 0 MEANS NO RELEASE
? .2,.2
INPUT CONTACT FACTORS FOR THE ACTIVE AND PASSIVE
STAGES - (0 TO 1) WHERE 1 IS MAXIMUM CONTACT.
? 0,1
INPUT CONTACT DURATION FACTORS FOR THE ACTIVE AND PASSIVE
STAGES - (MIN).
? 0,2000
INPUT SKIN AREA IN CONTACT WITH THE CHEMICAL DURING
THE ACTIVE AND PASSIVE EXPOSURE PERIODS - (0 TO 1)
WHERE 1 REFLECTS WHOLE BODY EXPOSURE.
? 0,.05
INPUT THE FRACTION OF THE MATERIAL ACTUALLY IN CONTACT
IN CONTACT WITH THE SKIN AT ANY GIVEN TIME FOR THE
ACTIVE AND PASSIVE STAGES (0 TO 1).
? .001
? .001
INPUT THE FRACTIONS OF SOLID LOST DURING THE ACTIVE,
PASSIVE AND PASSIVE-BYPASS STAGES OF ACTIVITY (0.0 TO 1.0)
? 0,.2,.1
INPUT THE CHARACTERISTIC EXPOSURE TIMES FOR THE
ACTIVE AND PASSIVE STAGES OF PRODUCT USE (HRS).
? 0,100000
INPUT THE EFFECTIVE DILUTION VOLUMES FOR THE ACTIVE
AND PASSIVE STAGES OF PRODUCT USE (M CUBED).
? 40,40

POPULATION      DOSE(KG)       TREL(SEC)      T-ACT(SEC)     T-PASS(SEC)
 0              0              2.45587E+08    0              3.60000E+08

 1              0              0
 2              5.184          3.88800E+09
 3              0              0
                               0
 5              0              4.32000E+08
```